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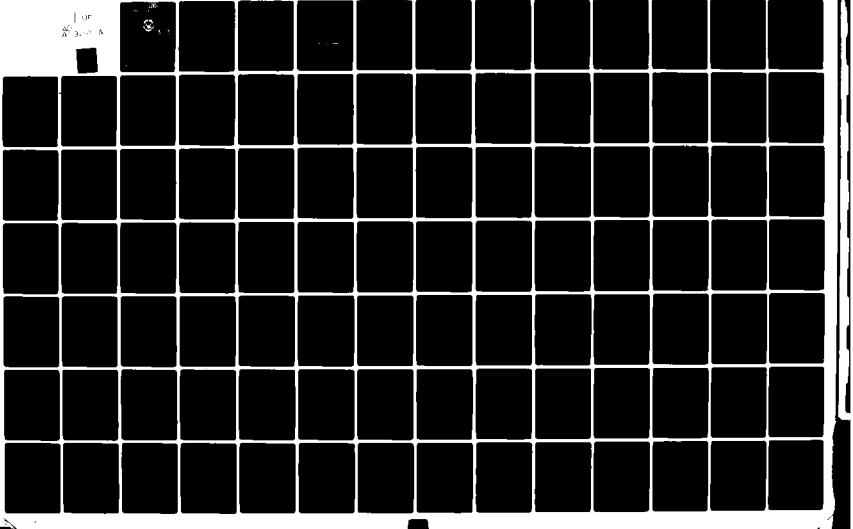

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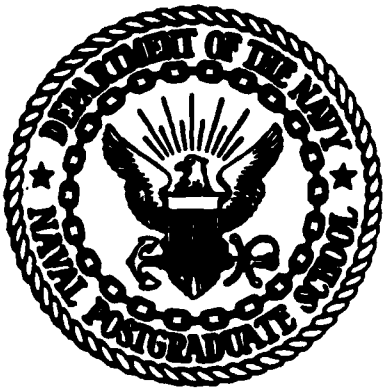

THESIS

ANALYSIS OF COMBUSTION AND HEAT TRANSFER
IN A POROUS GRAPHITE MEDIUM

by

Costa Sozon Vatikiotis

June 1980

Thesis Advisor: D. Salinas

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The problem of a porous graphite fiber plate subject to combustion is formulated. The transient one-dimensional model leads to two heat transfer equations on the graphite and air, and a mass transfer equation on the oxygen. In addition to a combustion heat generation term, the heat transfer model includes the mechanisms of conduction, radiation between fibers, and convection due to induced air flow through the mat. The mass transfer model

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Analysis of Combustion and Heat Transfer in a Porous Graphite Medium

by

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ABSTRACT

The problem of a porous graphite fiber plate subject to combustion is formulated. The transient one-dimensional model leads to two heat transfer equations on the graphite and air, and a mass transfer equation on the oxygen. In addition to a combustion heat generation term, the heat transfer model includes the mechanisms of conduction, radiation between fibers, and convection due to induced air flow through the mat. The mass transfer model includes diffusion and convection mechanisms, as well as a combustion consumption term. The temperature dependency of the system parameters is taken into account. The resulting nonlinear, coupled partial differential equations are solved by a Galerkin formulation of the finite element method. A number of computer analysis results are presented. The results show the effects of initial conditions, plate thickness, fiber diameter and air flow rate on ignition and extinction.

TABLE OF CONTENTS

LIST OF SYMBOLS

A^{-1} - characteristic time of reaction

$\underset{\sim}{A}$ - stiffness matrix

B - molecular diffusivity

$\underset{\sim}{B}$ - Gram matrix

c - specific heat at constant pressure

D - ply thickness

d - filament diameter

E - activation energy

e - element number

$\underset{\sim}{F}$ - excitation vector

f - stoichiometric ratio

G - global basis function

g - local basis function

Gr - Grashof number

G_o - pseudo mass velocity

h - convection heat transfer coefficient

$\hat{h}$ - specific enthalpy

ΔH - enthalpy of formation

J - Colburn j-factor

k - thermal conductivity

L - plate thickness

L* - reference length (= unity)

ℓ_e - element length

M - molecular weight

m - specific permeability

$\dot{m}$ - mass flow rate

n - number of nodal points

P - pressure

p - porosity

Pr - Prandtl number

q_g - heat generation

q_ℓ - heat loss

R - Universal Gas constant

R_A - gas constant for air

r - reaction rate

r_i - residual function

Re - Reynolds number

s - spacing between fibers

T - temperature

$\hat{T}$ - absolute temperature

t - time

U_∞ - flow over exterior surface

u_p - pore velocity

V - molecular volume

w - mean free path

x - one-dimensional coordinate

y - ratio of a fibers' surface area to its volume

z - ratio of fiber surface area per unit volume

Greek symbols

Γ - nondimensional air temperature

Δ - difference

δ - average pore diameter

δ_{ij} - kronecker delta

ε - emissivity

ξ - local coordinates

η - nondimensional length

Θ - nondimensional fiber temperature

Λ - spacial operator

λ - coefficient defined in Appendix A

μ - dynamic viscosity of air

ν - coefficient defined in Appendix A

ρ - density

σ - Stefan-Boltzmann constant

τ - tortuosity

Φ - nondimensional oxygen concentration

ϕ - oxygen concentration

Ψ - approximate solution values

Ψ_o - shape parameter for h_i

ω - coefficient defined in Appendix A; dummy variable

subscripts

a - air

B - diffusion

b - bulk property

c - convection

e - effective

f - fluid

g - fiber

i - internal

K - Kelvin

L - at x = L

O2 - oxygen

p - pore

r - radiation

s - solid

∞ - ambient condition

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I. INTRODUCTION

The combustion of a composite laminate plate consisting of graphite fibers in an epoxy matrix is discussed. The combustion process for a graphite laminate takes place in two stages, epoxy combustion followed by combustion of the graphite. At the end of the first stage the epoxy has burned away exposing a porous graphite mat. Spacing between the fibers is maintained by the residue of the combustion products. This present work is concerned with the last stage of the combustion process, specifically, the thermal response of the remaining graphite fiber mat.

The selection of the second stage for the analysis was made as a result of observations during composite plate "burn" experiments at the Naval Weapons Center, China Lake [1]. The objective of the experiments was to assess damage of composite aircraft structures subjected to open deck fires on aircraft carriers. For the experiments, an epoxy-graphite laminate was mounted into the wall of a wind tunnel parallel to the flow. One side of the composite plate was exposed to the wind tunnel flow and the opposite side was open to the environment. This arrangement was to simulate a composite wing section or fuselage subjected to typical wind conditions present on a carrier flight deck. It was observed that after being subjected to a fire which resulted in the

epoxy burning away, the graphite fibers would continue to smolder or burn. In other instances, the fibers would cool depending on the flow velocity and plate thickness. To understand this behavior better, a mathematical model was formulated to predict the conditions for which the exothermic process is self-sustaining.

The air flow over one surface produces a pressure differential across the plate which induces a convective air flow through the porous medium governed by Darcy's Law. As a result, there is an enhancement of internal convection heat transfer, as well as a source of oxygen for combustion. The heat transfer mechanisms included in the model are (1) conduction, (2) convection, and (3) radiation. In addition, non-volatile combustion is included in the energy balance as a heat generation term of Arrhenius type. The oxygen concentration is accounted for by a molecule-mass balance which includes (1) molecular diffusion, and (2) mass transfer by convection. Consumption of oxygen due to combustion is accounted for by a term similar to the heat generation term.

The formulation of a one-dimensional model is presented. All properties are treated as temperature dependent in the transient analysis. To account for heat transfer mechanisms between the air and porous graphite medium, the air and graphite temperatures are treated as independent variables. The energy balance on the graphite and on the air, and the

molecule-mass balance on oxygen result in a system of three nonlinear, coupled partial differential equations.

Integration of the field equations is accomplished by a Galerkin formulation of the finite element method. Due to the inherent stiffness of the field equations in the time domain, a modified implicit-Gear integration scheme developed by Franke [2] is used for a more efficient solution.

II. THEORY AND BACKGROUND

A. INTERACTION OF HEAT TRANSFER AND COMBUSTION

In this work, the combustion model proposed by Semenov was adopted. It is described in the texts of Frank-Kamenetskii [3] and Vulis [4]. A brief discussion of those features of the model which relate to the present investigation will be given. Fundamental to the model is the relation of reaction rate to temperature, and the interaction of the heat generation and the heat transfer from the system. In general, the reaction rate, r, may be shown by the Arrhenius law as,

$$r = A(T,\phi)\ \exp(-E/R\hat{T})$$

where A^{-1} is the characteristic time of the chemical reaction, E is the activation energy, R is the universal gas constant, $\hat{T}$ is absolute temperature and ϕ is the concentration of oxygen. The concentration appears as ϕ^n in $A(\hat{T},\phi)$ for an nth order reaction. The heat generated by the exothermic process is obtained by multiplying the reaction rate, r, by the enthalpy of formation of the combustion products.

In Figure 1, the heat generation, q_g, is plotted as a function of temperature. The curve is referred to as the S-curve for apparent reasons. The S-curves are distinguished

by two regions. Lower temperatures and reaction rates characterize region I, while region II is characterized by higher temperatures and reaction rates. In region I, for low reaction rates, there is an abundant supply of oxygen. The reaction is controlled by the temperature and the region is known as the kinetic regime. Here, the reaction rate increases exponentially with increasing temperature. In region II, the reaction is limited by oxygen concentration and is known as the diffusion regime. The reaction's weak dependence on temperature in region II is shown by the characteristic flattening of the S-curve in Figure 1. For higher concentrations of oxygen, the diffusion region is associated with higher reaction rates. The interaction of heat generation, q_g, and heat loss, q_ℓ, will now be described.

In addition to the S-curve, Figure 1 shows two heat loss lines, $q_{\ell 1}$ and $q_{\ell 2}$. They represent the heat transfer by convection for air temperatures, T_1 and T_2, respectively. The intersection of the heat generation curve and the heat loss curve, $q_g = q_\ell$, defines the stable quasi-stationary point, A. As the air flow temperature increases from T_1 to T_2, the quasi-stationary temperature increases continuously from T_A to T_I. For temperature T_I, $q_{\ell 2}$ is tangent to q_g and an infinitesimal increase in the air flow temperature results in a jump of the reaction temperature from T_I to T_B. At point I, which is defined as the "critical ignition condition", the reaction moves from the kinetic to the diffusion regime.

Temperature T_I is referred to as the ignition temperature. Frank-Kamenetskii states the ignition temperature of graphite is approximately 1100 to 1300 degrees Celsius. In order to keep the reaction model simple, the present investigation was limited to the kinetic regime. Although the description of the heat transfer process just presented is for convection only, the underlying ideas are valid for the conduction and radiation heat transfer mechanisms as well. The slope of the heat loss lines, q_ℓ, is equal to the product of the internal heat transfer coefficient and the surface area of fiber per unit volume. The slopes would not appear constant, and slight curvature in the heat loss lines, q_ℓ, is apparent when radiation effects are included. As shown in Figure 1, an increase in the heat transfer rate resulting, for example, by an increase in the internal flow rate would result in a lower graphite temperature for a given air temperature.

One reason for limiting the model to the kinetic regime was due to the jump in temperature and reaction rate at ignition. Though the discontinuity may be accounted for, the results show that for the region of temperatures approaching the diffusion regime, the heat generation will dominate the process. The system temperatures then rise rapidly. Other factors that limit the model to the lower temperatures are (1) the chemical reaction fixing the heat of combustion (complex at higher temperatures) and (2) the rapid consumption of fibers after ignition.

B. HEAT TRANSFER EQUATIONS FOR POROUS MEDIA

In their investigation of oil recovery from underground reservoirs, Green and Perry [5] developed heat transfer equations for the solid and fluid phases in a porous medium. Their model included the three basic mechanisms: (1) physical movement of the fluid which carries its own heat capacity, (2) conduction of heat through the solid and fluid phases, and (3) convective heat transfer between the solid and fluid phases. Radiation heat transfer was assumed to be negligible, and combustion was not a consideration. The differential equations for the fluid and solid phases

$$\text{Fluid:}\quad \rho_f c_f p \frac{\partial T_f}{\partial t} = -u\rho_f c_f p \frac{\partial T_f}{\partial x} + k_f p \frac{\partial^2 T_f}{\partial x^2} - hz(T_f - T_s) \qquad \text{(II.1)}$$

$$\text{Solid:}\quad \rho_s c_s (1-p) \frac{\partial T_s}{\partial t} = k_s (1-p) \frac{\partial^2 T_s}{\partial x^2} + hz(T_f - T_s) \qquad \text{(II.2)}$$

were solved numerically by the finite difference method. In equations II.1 and II.2, c is the specific heat at constant pressure, u is the fluid velocity through the medium, h is the coefficient of heat transfer, and k is a pseudothermal conductivity. The model did not include change of properties with temperature. Their numerical results showed good agreement with their experimental results. Two useful conclusions derived from their analysis were: (1) both conduction and convection heat transfer mechanisms are important for internal Reynolds numbers less than one, and (2) for values of the

dimensionless parameter, $\xi = (hz/k_f)^{1/2}(k_f/\rho_f c_f u)$ greater than .342, the fluid temperature is approximately the solid temperature. Riaz [6] proposed the following equation resulting from the equal fluid-solid temperature assumption,

$$\rho_s c_s \frac{\partial T}{\partial t} + \rho_f c_f u \frac{\partial T}{\partial x} = k_s \frac{\partial^2 T}{\partial x^2} \qquad \text{(II.3)}$$

where the coefficients are defined as those in equations II.1 and II.2. For the present model, the more general approach (i.e., Green and Perry) will be taken in the formulation of the energy equations.

III. FORMULATION OF THE FIELD EQUATIONS

A. INTERNAL FLOW MODEL

Referring to Figure 2, the porous mat may be represented by a flat plate. One side is exposed to still air, and the other to an air flow of velocity, U_∞. The environment on both sides is at ambient temperature, T_∞.

The first step in developing the model was to derive an expression for the flow through the porous plate. Effects of the combustion process on the physical properties were neglected. Specifically, these were (1) variations in the porosity due to fiber consumption, and (2) effects on the viscosity and density of air from the introduction of combustion by-products into the flow. Preliminary calculations showed that the porosity and density of the material did not change appreciably until temperatures reached approximately 2000 degrees Fahrenheit. Further, since eighty percent of air by volume is essentially inert, it was reasonable that its properties would not be significantly altered during the combustion process. Assuming a heterogeneous material of constant porosity, a Reynold's number for the interior flow is defined as

$$Re_i = \rho_a u_p d/\mu \qquad \text{(III.1)}$$

where ρ_a is the mass density of air, u_p is the pore velocity, d is the diameter of the fiber, and μ is the dynamic viscosity. Extensive experimental work shows that Darcy's law for flow through a porous medium is valid for a limited range of Reynolds numbers. Muskat [7] proposed that Darcy's flow is valid for $Re_i < 1$. Scheidegger [8] points out that a number of investigators give a much higher upper limit. Preliminary calculations of Re_i for the model showed typical magnitudes on the order of 1. Neglecting the gravity term, Darcy's law for flow in porous media is,

$$u_p = -\frac{m}{\mu}\frac{dP}{dx} \qquad \text{(III.2)}$$

assuming a constant pressure gradient, equation III.2 becomes,

$$u_p = -\frac{m}{\mu}\frac{\Delta P}{L} \qquad \text{(III.3)}$$

where ΔP is the pressure differential across the plate thickness, m is the specific permeability of the medium, and μ is the dynamic viscosity. In equations III.1 and III.3, ρ_a and μ were treated as temperature dependent.

Specific permeability is a measure of a porous medium's ability to allow fluid to flow through. It is dependent only on geometry and the physical nature of the medium. It has dimensions of length squared. Specific permeability is often

called the hydraulic conductivity due to the similarity of Darcy's law to that of Fourier's law for heat conduction. The permeability for a particular medium is normally measured by experimentation. However, there are several empirical models that may be used to obtain values for permeability that are in agreement with experimental results. For the idealized geometry of the porous medium shown in Figure 2, the permeability was obtained by a serial type model, equation III.4, proposed by Scheidegger [8],

$$m = \frac{1}{96} p (\delta/\tau)^2 \qquad \text{(III.4)}$$

where the porosity, p, is defined for a prous material comprised of fibers with cylindrical shape as,

$$p = 1 - \frac{\pi}{4}(d/D)^2 \qquad \text{(III.5)}$$

and D is the thickness of a ply. Porosity has units of volume of void per unit volume of medium. The average pore diameter, δ was defined as,

$$\delta = (s + D)/2$$

for the geometry in Figure 2. The tortuosity, τ, is a measure of length of travel for a fluid particle per unit thickness of the medium. Referring to the geometry of Figure 2, the

tortuosity depends on the ratio, d/D. The lower limit occurs when d/D equals zero and for the upper limit, d/D equals 1. Carman [9] presents a table of tortuosities for given geometries and particle shapes. For the model, Carman's suggested value of $\tau = 1.4$ was used.

To obtain the pressure differential, ΔP, across the porous plate, Bernoulli's equation was used. The following observations showed this to be a valid assumption. Schlichting [10] points out that for the ratio of u_p/U_∞ in the range of .0001 to .01, the effects of "blowing" or "suction" on the potential flow over the porous plate may be neglected. A typical value of u_p/U_∞ for the model at which $U_\infty = 25$ kt. was .0028. For steady flow over a flat plate, the flow field outside the boundary layer may be described by Bernoulli's equation. This is a direct result of the Navier-Stokes equation. In addition, the pressure gradient across the boundary layer may be taken equal to zero. Therefore, Bernoulli's equation (eq. III.6) may be used to obtain the pressure differential across the plate,

$$\int \frac{P}{\rho_a} dx + \frac{U^2}{2} = \text{constant.} \qquad \text{(III.6)}$$

The parameters in equation III.6 are defined as follows: P, pressure; ρ_a, the density of air; U, velocity of the air over the flat plate. For the model, the density of air was approximated by the Ideal Gas law as

$$\rho_a = P/R_a\hat{T}_a \qquad \text{(III.7)}$$

where R_a is the gas constant for air, $\hat{T}_a$ is the absolute temperature of air, and P is the pressure. Substituting this into equation III.6, gives

$$\int \left(\frac{R_a\hat{T}_a}{P}\right) dP + \frac{U^2}{2} = \text{constant}$$

and upon integrating, the expression becomes

$$R_a\hat{T}_a \ln P + \frac{U^2}{2} = \text{constant}$$

or,

$$R_a\hat{T}_{a1} \ln P_1 + \frac{U_1^2}{2} = R_a\hat{T}_{a2} \ln P_2 + \frac{U_2^2}{2}$$

Letting

$$P_1 = P_\infty, \quad U_1 = 0, \quad \hat{T}_{a1} = \hat{T}_{a2} = \hat{T}_\infty, \quad P_2 = P_L, \quad U_2 = U_\infty$$

and substituting these in above, yields

$$R_a\hat{T}_\infty \ln P_\infty = R_a\hat{T}_\infty \ln P_L + \frac{U_\infty^2}{2}$$

Rearranging the previous expression gives,

$$R_a \hat{T}_\infty \ln (P_\infty / P_L) = \frac{U_\infty^2}{2}$$

Taking the exponential of both sides and solving for P_L results in

$$P_L = P_\infty \exp (-U_\infty^2 / 2R_a \hat{T}_\infty)$$

From the above expression and noting that $\Delta P = P_L - P_\infty$, ΔP may be expressed as

$$\Delta P = P_\infty [\exp(-U_\infty^2 / 2R_a \hat{T}_\infty) - 1]$$

Darcy's law in approximate form (eq. III.3) for the model is

$$u_p = - \frac{m}{\mu} \frac{\Delta P}{L}$$

and substituting for ΔP, it follows that,

$$u_{p\infty} = \{\frac{m}{\mu} \frac{P_\infty}{L} [1 - \exp(-U_\infty^2 / 2R_a \hat{T}_\infty)]\} \qquad \text{(III.8)}$$

where

$$m = \frac{1}{96} P (\frac{\delta}{\tau})^2$$

The pore velocity, $u_{p\infty}$ of equation III.8 is for an isothermal medium at ambient temperature, T_∞. Since the model is to investigate the transient problem, a general expression to obtain pore velocity at different temperatures had to be developed.

Consideration of the continuity equation for one-dimensional steady flow,

$$d(\rho_a u_p)/dx = 0 \qquad \text{(III.9)}$$

becomes

$$u_p(d\rho_a/dx) + \rho_a(du_p/dx) = 0$$

or

$$u_p(d\rho_a/dx) = -\rho_a(du_p/dx)$$

Multiplying through both sides by dx, the expression becomes,

$$u_p d\rho_a = -\rho_a du_p$$

Separating variables and integrating both sides, gives

$$\int_{\rho_\infty}^{\rho_a} \frac{d\omega}{\omega} = - \int_{u_{p\infty}}^{u_p} \frac{d\omega}{\omega}$$

and the integral becomes

$$\ln(\rho_a/\rho_\infty) = \ln(u_{p\infty}/u_p)$$

Taking the exponential of both sides, gives

$$\rho_a/\rho_\infty = u_{p\infty}/u_p$$

Rearranging, the pore velocity is expressed as

$$u_p = p_\infty u_{p\infty}/\rho_a \qquad \text{(III.10)}$$

Referring to the Ideal Gas law for the density of air, and substituting this into equation III.10 gives

$$u_p = (\rho_\infty u_{p\infty} R_a \hat{T}_a)/P \qquad \text{(III.11)}$$

The pore velocity is now a function of air temperature and pressure. However, in preliminary calculations, the pressure difference, ΔP was small and for the range of parameters of interest, it did not exceed five percent of the magnitude of ambient pressure. Therefore, as a simplification, it was assumed that P equals the ambient pressure in equation III.11,

and the expression becomes

$$u_p = (\rho_\infty u_{p\infty} R_a \hat{T}_a)/P_\infty$$

Noting that $\rho_\infty = P_\infty/R_a T_\infty$, the pore velocity may be expressed as

$$u_p = u_{p\infty} \hat{T}_a/\hat{T}_\infty \qquad \text{(III.12)}$$

where $u_{p\infty}$ is obtained from equation III.8. $\hat{T}_a$ and $\hat{T}_\infty$ are the absolute temperatures of the air at a point in the interior of the medium and of the environment, respectively.

B. ENERGY EQUATIONS

Here we consider the development of the energy equations. However, before continuing, discussion must be made as to the approach taken for energy balances in porous media. In previous work by Denbigh and Turner [11], and by Colladay and Stepka [12], it was suggested that the temperature of the porous solid and of the fluid be considered equal. This greatly simplifies the formulation of the problem. However, under certain conditions, as shown by Green and Perry [5], the assumption of equal temperatures may not be valid. With recent developments in numerical techniques permitting the solution of non-linear systems, the development of the present model for heat transfer in a porous medium was not restricted

to the assumption of equal temperatures. Therefore, the temperatures of the air and of the porous solid are treated as independent variables in the present formulation.

The model is based on two assumptions. First, due to the small thickness of the graphite fibers, the temperature across each individual fiber was assumed to be constant. Second, for a similar size consideration, the temperature of the air in each individual pore was assumed constant. However, the temperature from fiber to fiber and from pore to pore was not restricted, and was allowed to vary according to the heat transfer mechanisms described next.

To perform energy balances on both the porous solid and on the air, a differential volume of porous material was segregated into respective volumes of constituents, that is, graphite fibers and air (Figure 3). An energy balance may be done on each volume separately. The convention used for the balance is:

$$\begin{matrix}\text{Heat into} \\ \text{dV}\end{matrix} + \begin{matrix}\text{Heat} \\ \text{Generation}\end{matrix} = \begin{matrix}\text{Heat out} \\ \text{of dV}\end{matrix} + \begin{matrix}\text{Increase in} \\ \text{Internal} \\ \text{Energy}\end{matrix}$$

where

$$dV = dx\, dy\, dz$$

1. Fiber Heat Transfer Equation

Considering the differential volume, (1-p)dV of graphite fibers, and "smearing" the fibers to form a macroscopically homogeneous material, the heat transfer mechanisms are shown for the x-direction in Figure 4. The heat transfer mechanisms are: q_{cond}, heat conduction through the medium; q_{conv}, convection from the fibers to the air; q_{rad}, radiation transfer from fiber to fiber; $\Delta Hr(T_g,\phi)$ heat generation rate per unit volume. ΔH is the enthalpy of formation, and $r(T_g,\phi)$ is the fiber mass consumption rate. This term will be discussed in detail later.

Representing the terms in Figure 4 by Taylor series expansions and combining them with respect to the convention previously stated, the energy balance is

$$q_{cond} + q_{rad} + \Delta Hr(T_g,\phi)(1-p)dxdydz = q_{cond} + \frac{\partial q_{cond}}{\partial x} dx$$

$$+ q_{rad} + \frac{\partial q_{rad}}{\partial x} dx + q_{conv} + \frac{\partial E}{\partial t}(1-p)dxdydz$$

Subtracting terms, q_{cond} and q_{rad} from each side and rearranging, the expression becomes (neglecting the higher order terms)

$$-\frac{\partial q_{cond}}{\partial x} dx - \frac{\partial q_{rad}}{\partial x} - q_{conv} + \Delta Hr(T_g,\phi)(1-p)dxdydz$$

$$= \frac{\partial E}{\partial t}(1-p)dxdydz \qquad \text{(III.13)}$$

The heat transfer terms in equation III.13 will now be considered.

a. Thermal Conduction

Fourier's law for conduction may be written for the incremental volume as

$$q_{cond} = - k_g \frac{\partial T_g}{\partial x} dydz \qquad \text{(III.14)}$$

where k_g is the effective conductivity of the porous solid, and T_g is the temperature of the fibers. There are a variety of models for the effective conductivities of porous media. They depend largely on the geometry and on the nature of the constituents. For the cylindrical shape of the fibers, the empirical relation proposed by Rohsenow [13] was used

$$k_g = k_a\{1-\beta[1 + \frac{\gamma}{(1-\gamma)^{1/2}} \ln(\frac{1-(1-\gamma^2)^{1/2}}{\gamma})]\} \qquad \text{(III.15)}$$

for $\gamma^2 < 1$. The parameters of equation III.15 are defined as follows: $\beta = d/D$ (refer to Figure 2), γ is

$$\gamma = \frac{1}{\beta}[\frac{\Lambda}{(1-\Lambda)}]$$

where $\Lambda = k_a/k_g'$, k_a is the conductivity of the air; and k_g' is the actual conductivity of the graphite in bulk form. Since k_a depends on temperature, k_g was also treated as temperature dependent.

b. Radiation Heat Transfer in Fibers

Radiation heat transfer in the model was represented by an analog to Fourier's law of conduction as

$$q_{rad} = - k_r \frac{\partial T_g}{\partial x} dy\ dz \qquad \text{(III.16)}$$

where k_r is an equivalent conductivity of the fibers due to radiation. Simple assumptions and approximations may be made to show this. Assuming air to be transparent to radiation, and treating a ply of graphite fibers as an infinite wall, the net heat flux between plies may be written as

$$q''_{rad} = \frac{\sigma\varepsilon}{(2-\varepsilon)}(\hat{T}^4_{gx} - \hat{T}^4_{gx+dx}) \qquad \text{(III.17)}$$

where $\hat{T}_{gx}$ and $\hat{T}_{gx+dx}$ are the respective absolute ply temperatures, ε is the emissivity of the graphite, and σ is the Stefan-Boltzman constant. Treating T_{gx} as the variable temperature, q''_{rad} may be expanded in a Taylor series about $\hat{T}_{gx+dx}$. Neglecting the higher order terms, the series expansion may be written as

$$q''_{rad} = \frac{\sigma\varepsilon}{2-\varepsilon}(\hat{T}^4_{gx+dx} - \hat{T}^4_{gx+dx}) + \frac{4\sigma\varepsilon}{2-\varepsilon}\hat{T}^3_{gx+dx}(\hat{T}_{gx} - \hat{T}_{gx+dx})$$

Simplifying, the above equation becomes,

$$q''_{rad} = \frac{4\sigma\varepsilon}{2-\varepsilon}\hat{T}^3_{gx+dx}(\hat{T}_{gx} - \hat{T}_{gx+dx}) \qquad \text{(III.18)}$$

Taking Fourier's law for heat transfer,

$$q''_{rad} = - k_r \frac{dT_g}{dx}$$

and approximating $\frac{dT_g}{dx}$ with

$$\frac{dT_g}{dx} = \frac{\Delta \hat{T}_g}{\Delta x} = \frac{\hat{T}_{gx+dx} - \hat{T}_x}{\Delta x}$$

q''_{rad} becomes

$$q''_{rad} = - k_r \frac{(\hat{T}_{gx+dx} - \hat{T}_{gx})}{\Delta x} \qquad \text{(III.19)}$$

Multiplying the right side of equation III.18 by $\Delta x/\Delta x$, equation III.18 and equation III.19 may be equated

$$q''_{rad} = - k_r \frac{(\hat{T}_{gx+dx} - \hat{T}_{gx})}{\Delta x} = - \frac{4\sigma\varepsilon\Delta x}{2-\varepsilon} \hat{T}^3_{gx+dx} \frac{(\hat{T}_{gx+d\bar{x}} - \hat{T}_{gx})}{\Delta x}$$

Cancelling terms, k_r becomes

$$k_r = \frac{4\sigma\varepsilon\Delta x}{2-\varepsilon} \hat{T}^3_{gx+dx} \qquad \text{(III.20)}$$

where Δx is now equal to δ, the average pore diameter. From the close spacing of the fiber layers, the temperature difference will be small as compared to the magnitude of the temperature. Noting this the average absolute temperature of

the fibers, $\hat{T}_g$ may be substituted for $\hat{T}_{gx+dx}$. The equivalent radiation conductivity expression becomes

$$k_r = \frac{4\sigma\varepsilon\delta}{2-\varepsilon} \hat{T}_g^3 \qquad \text{(III.21)}$$

and the radiation heat transfer from fiber to fiber may be represented by,

$$q_{rad} = - k_r \frac{\partial T_g}{\partial x} = - \frac{4\sigma\varepsilon\delta}{2-\varepsilon} \hat{T}_g^3 \frac{\partial T_g}{\partial x} \, dy \, dz \qquad \text{(III.22)}$$

If the temperature gradient in the fibers is not large, then equation III.22 will be a good approximation of the radiation heat transfer between the fibers.

c. Convection Heat Transfer

The convection heat transfer term in Figure 4 was treated in a similar manner to that of the one-dimensional fin equation. q_{conv} was introduced as

$$q_{conv} = h_i (T_g - T_a) \, dA \qquad \text{(III.23)}$$

where T_g is the temperature of the graphite, T_a is the temperature of the air, dA is the surface area of graphite in the differential volume, and h_i is the internal convection heat transfer coefficient. An empirical expression in the form of a Colburn j-factor was developed by Yoshida, Ramaswami, Hougen [14]. This was used to determine h_i,

$$J = \frac{h_i}{c_b G_o}\left[\frac{c_a \mu}{k_a}\right]^{2/3} = .91\ Re^{-.51}\psi_o \qquad (III.24)$$

for Re < 50. c_b is the effective specific heat of the porous medium and is defined as,

$$c_b = pc_a + (1-p)c_g$$

where c_a is the specific heat of air at constant pressure; c_g is the specific heat of graphite; and p is the porosity as defined by equation III.5. G_o is a pseudo mass velocity defined as $G_o = \rho_a u_p p$. Also in equation III.24, μ is the viscosity of air, and k_a is the conductivity of air. The Reynolds number appearing in equation III.24 is defined as

$$Re = G_o/z\ \mu\ \psi_o$$

and is not the same as Re_i defined previously for Darcy's law. z is the surface area of graphite fibers per unit volume, and is determined from geometrical considerations which will be described shortly. The parameter, ψ_o, is a dimensionless shape factor which depends on the geometry of the fibers. For a cylindrical fiber shape, ψ_o is equal to .91. From the assumption of constant porosity, z remains constant. However, the air properties are temperature dependent; therefore, h_i is allowed to vary with temperature.

d. Heat Generation Rate

The reaction rate, $r(T_g,\phi)$, whether based upon the Collision Theory or on the Theory of Absolute Reaction Rates, results in an expression of Arrhenius type,

$$r = A(\hat{T},\phi)\ \exp(-E/R\hat{T})$$

where E is the activation energy, R is the universal gas constant, and $\hat{T}$ is absolute temperature. Although E is well defined for the combustion of graphite, $A(\hat{T},\phi)$ is a function of temperature and concentration and depends upon chemical kinetic theory. Development of a general model for the chemical kinetics is beyond the scope of this work. A less elegant, but useful approach of using a relation obtained experimentally was taken. A relation derived from the work of Parker and Hottel [15] was used to predict the combustion rate of graphite fibers,

$$r = 4.014 \times 10^7\ R_A\ \hat{T}_g^{1/2}\ y\ \phi\ \exp\left(\frac{-39,883}{\hat{T}_g}\right)\ \frac{\text{lbm}}{\text{ft}^3\text{-hr}} \qquad \text{(III.25)}$$

The development of equation III.25 from the original work may be found in the appendix. This expression assumes a simple first-order reaction for the combustion of graphite in air. However, Frank-Kamenetskii [3] has further refined Parker and Hottel's expression to yield for the present model,

$$r = 4.014 \times 10^7 R_A T_g^{1/2} y \phi^n \exp\left(\frac{-39,883}{\hat{T}_g}\right) \quad \frac{lbm}{ft^3\text{-}hr} \qquad \text{(III.26)}$$

The combustion is now characterized as an nth order reaction, where n is in the range of 1/3 to 2/3. This form of the reaction rate expression better approximates Parker and Hottel's experimental data. For the analysis, n was chosen to be 1/2. However, it should be pointed out that the behavior of the reaction varies significantly within the range of n proposed by Frank-Kamenetskiii.

In limiting the model to the kinetic regime of combustion, it was assumed that the dominant chemical reaction is

$$C + O_2 \longrightarrow CO_2$$

This is an idealized treatment of the reaction that actually takes place. Kanury [16] states that, the actual reaction is more complex, yielding various concentrations of carbon dioxide and carbon monoxide, depending on the temperature. Noting the abundant oxygen supply present in the kinetic regime, it is reasonable that the leaner oxide is the prevalent by-product of combustion. The fuel-oxygen ratio, f, for this mechanism is 12/32. Carbon monoxide may be formed when there is little free-oxygen present, such as, during combustion in the diffusion regime. The stoichiometric

fuel-oxygen ratio, f = 12/16, for this mechanism is naturally greater. To obtain the heat generation rate, the reaction rate, r, was multiplied by the enthalpy of formation, ΔH, of carbon dioxide. ΔH has units of Btu per lbm of graphite consumed.

e. Change in Internal Energy

The last term of the graphite energy equation, the rate of change of internal energy, $\frac{\partial E}{\partial t}$, results by setting $E = \rho_g c_g T_g$. Thus,

$$\frac{\partial E}{\partial t}(1-p)dxdydz = (1-p)\rho_g c_g \frac{\partial T_g}{\partial t} dxdydz \qquad \text{(III.27)}$$

where ρ_g is the density of graphite in bulk; c_g is the specific heat of graphite; and p is the porosity.

The heat transfer mechanisms for the graphite fibers, equations III.14, III.16, III.23, III.26, III.27 are substituted into equation III.13 which upon dividing through by dV = dxdydz yields the heat transfer equation for the fibers,

$$(1-p)\frac{\partial}{\partial x}(k_g \frac{\partial T_g}{\partial x}) + (1-p)\frac{\partial}{\partial x}(k_r \frac{\partial T_g}{\partial x}) - h_i \frac{dA}{dV}(T_g - T_a)$$

$$+ (1-p)\Delta Hr(T_g, \phi) = (1-p)\rho_g c_g \frac{\partial T_g}{\partial t}$$

The coefficient, (1-p), accounts for the fact that not all of the volume of porous medium is comprised of graphite.

Dividing through by (1-p), combining the first two terms, and defining dA/dV as z, the surface area of graphite per unit volume, the expression becomes

$$\frac{\partial}{\partial x}[(k_g + k_r)\frac{\partial T_g}{\partial x}] - \frac{h_i z}{(1-p)}(T_g - T_a) + \Delta Hr(T_g,\phi)$$

$$= \rho_g c_g \frac{\partial T_g}{\partial t} \qquad \text{(III.28)}$$

The parameter, z, is obtained from geometry considerations. For a cylindrical fiber shape, the expression for z is,

$$z = \pi d/2D^2 \qquad \text{(III.29)}$$

The one-half factor in equation III.29 accounts for the uncertainty of the actual amount of exposed fiber surface area, which resulted from the initial combustion of epoxy. The non-dimensionalization of equation III.28 is presented in Appendix A.

2. Internal Flow Heat Transfer Equation

The energy balance on the internal flow is obtained by a procedure similar to the energy balance on graphite. Figure 5 presents a "smeared" differential volume of air, pdV, which shows the heat transfer mechanisms. The heat transfer mechanisms are: q_{cond}, heat conduction through the air; q_{conv}, convection from the fibers to the air; $\dot{m}_a \hat{h}$,

energy transport due to the air flow, where $\hat{h}$ is the enthalpy of the air.

Performing the energy balance (neglecting the higher order terms) yields,

$$q_{cond} + \dot{m}_a \hat{h} + q_{conv} = q_{cond} + \frac{\partial q_{cond}}{\partial x} dx + \dot{m}_a \hat{h} + \dot{m}_a \frac{\partial h}{\partial x} dx + \frac{\partial E}{\partial t} pdxdydz \qquad \text{(III.30)}$$

Cancelling terms and rearranging, the expression becomes,

$$- \frac{\partial q_{cond}}{\partial x} dx - \dot{m}_a \frac{\partial \hat{h}}{\partial x} dx + q_{conv} = \frac{\partial E}{\partial t} pdxdydz \qquad \text{(III.31)}$$

a. Thermal Conduction

As before, q_{cond} was replaced by Fourier's law of heat conduction in the form,

$$q_{cond} = - k_a \frac{\partial T_a}{\partial x} dydz \qquad \text{(III.32)}$$

where k_a is the conductivity of air.

b. Energy Transport by Flow

Using the perfect gas assumption for air, the enthalpy $\hat{h}$ was expressed as,

$$d\hat{h} = c_a \, dT_a$$

where c_a is the specific heat of air at constant pressure. The specific heat is treated as constant since it does not vary appreciably over the range of temperatures associated with the problem under investigation. It follows that,

$$\frac{\partial \hat{h}}{\partial x} = c_a \frac{\partial T_a}{\partial x} \qquad \text{(III.33)}$$

Assuming the effects of the combustion by-products on air are negligible, continuity considerations give the mass flow as,

$$\dot{m}_a = \rho_{a_\infty} u_{p_\infty} dydz \qquad \text{(III.34)}$$

where the density of air and the pore velocity are evaluated at ambient conditions.

c. Convection Heat Transfer

The convection heat transfer, q_{conv} given by equation III.23, with h_i obtained from equation III.24, becomes

$$q_{conv} = h_i(T_g - T_a)dA \qquad \text{(III.35)}$$

d. Change in Internal Energy

For a perfect gas, the internal energy is,

$$dE = \rho_a c_a dT_a$$

where c_a is the specific heat of air at constant pressure. From this it follows that

$$\frac{\partial E}{\partial t} p \, dxdydz = \rho_a c_a \frac{\partial T_a}{\partial x} p \, dxdydz \qquad \text{(III.36)}$$

Substituting equations III.32-III.36 into equation III.31, the heat transfer equation for the internal flow becomes,

$$\frac{\partial}{\partial x}(k_a \frac{\partial T_a}{\partial x}) pdxdydz - \dot{m}_a c_a \frac{\partial T_a}{\partial x} p \, dxdydz$$

$$+ h_i \, dA(T_g - T_a) = \rho c_a \frac{\partial T_a}{\partial t} p \, dxdydz$$

As in the energy equation for the fibers, the porosity, p, accounts for the fact that some of the volume of the porous medium is not air. Dividing the last equation through by pdxdydz and letting z denote dA/dxdydz, yields

$$\frac{\partial}{\partial x}(k_a \frac{\partial T_a}{\partial x}) - \dot{m}_a c_p \frac{\partial T_a}{\partial x} + \frac{h_i z}{p}(T_g - T_a)$$

$$= \rho_a c_a \frac{\partial T_a}{\partial t} \qquad \text{(III.37)}$$

Non-dimensionalization of equation III.37 may be found in Appendix A.

3. Oxygen Transport Equation

The final consideration in the formulation of the model is the mass transport of oxygen. The mass transport equation is obtained by a mass balance on a differential volume of porous medium. In accordance with convention, the mass balance is given by

$$\text{Oxygen into dV} = \text{Oxygen out of dV} + \text{Oxygen Consumption} + \text{Oxygen Accumulation}$$

Figure 6 presents a differential volume, pdV, showing the relevant molecule-mass transport mechanisms. The mass transport mechanisms are: $\dot{m}_B$ is the molecular diffusion; $\dot{m}_C$ is the convective transport due to mass flow; $\frac{1}{f}r(T_g,\phi)$ is the consumption of oxygen due to combustion; r is the reaction rate, and f is the stoichiometric ratio of the reaction. Representing the terms in Figure 6 by Taylor series expansions, the molecule-mass balance becomes (neglecting higher order terms),

$$\dot{m}_B + \dot{m}_C = \dot{m}_B + \frac{\partial \dot{m}_B}{\partial x}dx + \dot{m}_C + \frac{\partial \dot{m}_C}{\partial x}dx$$

$$+ \frac{1}{f}r(T_g,\phi)pdxdydz + \frac{\partial \phi}{\partial t}pdxdydz \qquad \text{(III.38)}$$

Upon cancelling terms and rearranging, equation III.38 becomes

$$- \frac{\partial \dot{m}_B}{\partial x} dx - \frac{\partial \dot{m}_C}{\partial x} dx - \frac{1}{f} r(T_g, \phi) p dx dy dz = \frac{\partial \phi}{\partial t} p dx dy dz \quad \text{(III.39)}$$

where ϕ is the concentration of oxygen. The individual mass transfer terms in equation III.39 will now be developed.

a. Molecular Diffusion

Molecular diffusion $\dot{m}_B$, is given by Fick's law,

$$\dot{m}_B = - B \frac{\partial \phi}{\partial x} dy\ dz \quad \text{(III.40)}$$

where B is the diffusivity of oxygen into the porous medium.

The diffusion of gases in porous media is limited by two factors. One is the collision of the gas molecules with other molecules, and the second is the collision of the gas molecules with the solid pore walls. This second phenomenon is discussed by Bennett and Myers [17] and is referred to as Knudsen diffusion. To establish which behavior dominates, the mean free path of the gas (in this case, oxygen), must be calculated. Using the expression given by Treybal [18],

$$w = (3.2\mu/P)(R\hat{T}/2\pi g_c M)^{1/2}$$

where g_c is the gravitational constant, the value obtained for mean free path, w, is smaller than 0.1δ. Thus, the collision of the oxygen molecules with those of air will restrict the diffusion process. On the contrary, if the pore

diameter is smaller than the mean free path, then the collision of the molecules with the solid walls will be the limiting factor. In the intermediate case, the mean free path and the pore diameter are of the same order of magnitude. In this case, Bennett and Myers [17] proposed the following expression be used to obtain a value of diffusivity,

$$\frac{1}{B_R} = \frac{1}{B_g} + \frac{1}{B_w} \qquad \text{(III.41)}$$

where B_R is the resulting diffusivity; B_g is the diffusivity based on molecule-molecule collisions; and B_w is the diffusivity based on molecule-pore wall collisions.

For the problem under investigation here, preliminary calculations of the mean free path of the oxygen showed that diffusion is primarily of the inter-molecular collision type. With respect to this, and knowing that molecular diffusion is highly temperature dependent, the diffusivity, B* was obtained from an expression presented by Gilliland [19].

$$B^* = 435.7 \frac{\hat{T}_a^{3/2}}{P}(V_a^{1/3} + V_{02}^{1/3})^{-2}(M_a^{-1} + M_{02}^{-1})^{1/2} \quad cm^2/s \qquad \text{(III.42)}$$

where P is the absolute pressure; V_a and V_{02} are the molecular volumes of air and oxygen respectively; M_a and M_{02} are the molecular weights of air and oxygen, respectively, and B* is the diffusivity. For this expression, $\hat{T}_a$ is in degrees

Kelvin, and B* has the units of cm^2/s. As a result of tortuosity and porosity affecting the process, Denbigh and Turner [11] proposed that the effective molecular diffusivity for a porous medium is given by

$$B_e = pB^*/\tau.$$

The porosity p accounts for the void in a differential cross-section.

b. Convective Transport

The convective term in equation III.39 is given by

$$\dot{m}_c = pu_p \phi dydz \qquad \text{(III.43)}$$

The pore velocity u_p is a temperature dependent variable, and is so treated.

c. Consumption Rate

The reaction rate term, $r(T_g, \phi)$ was discussed previously as equation III.26. The consumption rate of oxygen is determined by multiplying r by 1/f.

Substituting equations III.40 and III.43 into equation III.39, the oxygen transport equation becomes,

$$\frac{\partial}{\partial x}\left(\frac{B^*}{\tau}\frac{\partial \phi}{\partial x}\right) pdxdydz - \frac{\partial}{\partial x}(u_p \phi)\, pdxdydz$$

$$- \left(\frac{1}{f}\right) r(T_g, \phi) pdxdydz = \frac{\partial \phi}{\partial t} pdxdydz$$

Dividing both sides by pdxdydz, and letting $B = B^*/\tau$, the expression becomes

$$\frac{\partial}{\partial x}(B \frac{\partial \phi}{\partial x}) - \frac{\partial}{\partial x}(u_p \phi) - (\frac{1}{f}) r(T_g, \phi) = \frac{\partial \phi}{\partial t} . \qquad \text{(III.44)}$$

Expanding the second term of equation III.44,

$$\frac{\partial}{\partial x}(u_p \phi) = u_p \frac{\partial \phi}{\partial x} + \frac{\partial u_p}{\partial x} \phi$$

and noting that u_p depends on T_a from equation III.12, the expression yields

$$\frac{\partial}{\partial x}(u_p \phi) = u_p \frac{\partial \phi}{\partial x} + \frac{\partial u_p}{\partial T_a} \frac{\partial T_a}{\partial x} \phi . \qquad \text{(III.45)}$$

$\partial u_p / \partial T_a$ is obtained from equation III.12.

Substituting equation III.45 into equation III.44, the oxygen transport equation becomes,

$$\frac{\partial}{\partial x}(B \frac{\partial \phi}{\partial x}) - u_p \frac{\partial \phi}{\partial x} - \frac{\partial u_p}{\partial T_a} \frac{\partial T_a}{\partial x} \phi - (\frac{1}{f}) r(t_g, \phi) = \frac{\partial \phi}{\partial t} \qquad \text{(III.46)}$$

In contrast with the heat transfer equations, mass balance does not depend on porosity. However, porosity does influence the oxygen concentration by appearing in the boundary conditions. Non-dimensionalization of equation III.46 is presented in Appendix A.

IV. BOUNDARY CONDITIONS

It was intended that boundary conditions be imposed which simulate the composite plate "burn" experiments of Fontenot [1]. However, for a one-dimensional model, the boundary conditions can only be approximated at best. The difficulty is associated with the existence of momentum and thermal boundary layers on the exterior surface of the porous plate. Complications also arise from the "blowing and suction" effects which are caused by the flow through the plate.

The following boundary conditions provide a reasonable model for the one-dimensional problem,

$$(k_g + k_r)\frac{\partial T_g}{\partial x} = h_1(T_g - T_\infty) + \sigma\varepsilon(\hat{T}_g^4 - \hat{T}_\infty^4) \quad \text{at} \quad x = 0 \qquad \text{(IV.1)}$$

$$(k_g + k_r)\frac{\partial T_g}{\partial x} = -h_2(T_g - T_\infty) - \sigma\varepsilon(\hat{T}_g^4 - \hat{T}_\infty^4) \quad \text{at} \quad x = L \qquad \text{(IV.2)}$$

$$T_a = T_\infty \quad \text{at} \quad x = 0 \qquad \text{(IV.3)}$$

$$\frac{\partial T_a}{\partial x} = \frac{\partial T_g}{\partial x} \quad \text{at} \quad x = L \qquad \text{(IV.4)}$$

$$B\frac{\partial \phi}{\partial x} = u_p(\phi - p\phi_\infty) \quad \text{at} \quad x = 0 \qquad \text{(IV.5)}$$

$$\frac{\partial \phi}{\partial x} = 0 \quad \text{at} \quad x = L \qquad \text{(IV.6)}$$

Boundary conditions IV.1 and IV.2 account for convection and radiation heat transfer from the porous solid. With an influx of air at x = 0, the heat transfer coefficient, h_1, will depend on the magnitude of the flow entering the plate. Neglecting "blowing and suction" effects, several empirical expressions based on free convection were used to obtain a heat transfer coefficient at x = 0. These expressions yielded a range of values for h_1 from 1 to 3 Btu/hr·ft^2·F. As an approximation, h_1 was taken as the average value, 2.0 Btu/hr·ft^2·F. However, choosing h_1 as any value in the above range did not affect the results of the analysis.

The magnitude of the forced convection heat transfer coefficient at x = L, h_2, varies in a direction parallel to that of the external flow, U_∞. In addition, h_2 depends on the efflux of the gas at the surface. To simplify the analysis, h_2 was approximated by the relation for a smooth flat plate given by Holman [20] as

$$h_2 = .664 \frac{k_a}{L^*} Pr^{1/3} Re^{1/2} \qquad (IV.7)$$

for laminar flow, where Pr is the Prandtl number and L* is a reference length, arbitrarily taken as unity. For turbulent flow,

$$h_2 = \frac{k_a}{L^*} Pr^{1/3}(.037 Re^{.8} - 850). \qquad (IV.8)$$

Kays [21] provides an alternate scheme for treating boundary layers and "blowing and suction" effects.

Boundary condition IV.3 accounts for the air entering the porous plate at ambient temperature. The Dankwerts boundary condition proposed by Riaz [6] which accounts for conduction-convection interaction, is a more reasonable simulation.

The boundary condition at x = L for the air heat transfer equation appears to be a reasonable one. It follows the behavior observed in the interior of the plate and does not fix the temperature of the air at the wall. The boundary condition, $\partial T_a/\partial x = 0$, used initially provided results similar to those obtained using equation IV.4.

Boundary conditions IV.5 and IV.6 are Dankwert conditions [22] for flow through porous media. A convincing discussion for the Dankwerts conditions is given by Bischoff [23]. A brief summary of the discussion is presented in Appendix D.

V. FINITE ELEMENT METHOD

A. GALERKIN FORMULATION

A Galerkin formulation of the Finite Element Method was used to obtain solutions of the field equations. A convenient form of the field equations was used in the formulation. These equations are presented in Appendix A.

graphite energy equation

$$\frac{\partial}{\partial \eta}(\lambda_1 \frac{\partial \Theta}{\partial \eta}) - \lambda_2(\Theta - \Gamma) + \lambda_3 r(T_g, \phi) = \lambda_4 \frac{\partial \Theta}{\partial t} \quad (V.1)$$

air energy equation

$$\frac{\partial}{\partial \eta}(\nu_1 \frac{\partial \Gamma}{\partial \eta}) - \nu_2 \frac{\partial \Gamma}{\partial \eta} + \nu_3(\Theta - \Gamma) = \nu_4 \frac{\partial \Gamma}{\partial t} \quad (V.2)$$

oxygen diffusion equation

$$\frac{\partial}{\partial \eta}(\omega_1 \frac{\partial \phi}{\partial \eta}) - \omega_2 \frac{\partial \phi}{\partial \eta} - \omega_3 \frac{\partial \Gamma}{\partial \eta} \phi - \omega_4 r(T_g, \phi) = \omega_5 \frac{\partial \phi}{\partial t} \quad (V.3)$$

where the coefficients are defined in Appendix A.

Field equations III.28, III.37 and III.46 subject to boundary conditions, IV.1 - IV.6, and initial conditions define the problem. The closed domain (0,L) was partitioned into (n-1) contiguous elements of variable length ℓ_i, i = 1, ...,(n-1). This defines an n nodal point model. The three

non-dimensional field variables Θ, Γ, Φ were approximated by

$$\Theta(\eta,t) \tilde{=} \Psi_1(\eta,t) = \sum G_i(\eta)\Theta_i(t) \qquad (V.4)$$

$$\Gamma(\eta,t) \tilde{=} \Psi_2(\eta,t) = \sum G_i(\eta)\Gamma_i(t) \qquad (V.5)$$

$$\Phi(\eta,t) \tilde{=} \Psi_3(\eta,t) = \sum G_i(\eta)\Phi_i(t) \qquad (V.6)$$

where G_i, for $i = 1, \ldots, n$, is a set of specified basis functions with local support, and the sets $\{\Theta_i, \Gamma_i, \Phi_i; i = 1, \ldots, n\}$ are the solution coefficients to be determined. The G_i were selected to satisfy the condition $G_i(\eta_j) = \delta_{ij}$, where the kronecker delta δ_{ij} is defined by $\delta_{ij} = 1$ for $i = j$, and $\delta_{ij} = 0$ for $i \neq j$. As a result, Θ, Γ, and Φ are the values Ψ_1, Ψ_2, Ψ_3 at the nodal points (i.e., $\Theta_i(t) = \Psi_1(\eta_i,t)$).

Linear interpolation functions (Figure 7) were used as the basis functions. These are the lowest polynomial functions which provide the necessary function continuity.

As a measure of error, a residual function, r_i, is defined for each field equation by

$$r_i(\eta,t) = \Lambda_i(\underset{\sim}{\Psi}) - \dot{\Psi}_i \quad i = 1, 2, 3 \qquad (V.7)$$

where Λ_i denotes the spatial operator of the ith equation. For convenience, the following convention for differentiation

is adopted,

$$\frac{\partial(\ )}{\partial \eta} = (\ )'$$

$$\frac{\partial^2(\ )}{\partial \eta^2} = (\ )''$$

$$\frac{\partial(\ )}{\partial t} = (\dot{\ })$$

For field equations V.1, V.2, and V.3 the residuals are:

$$r_1 = [\lambda_1(\underset{\sim}{\Theta},\underset{\sim}{\Gamma}) \sum_{i=1}^{n} G_i'\Theta_i]' - \lambda_2(\underset{\sim}{\Gamma}) \sum_{i=1}^{n} G_i(\Theta_i - \Gamma_i)$$

$$+ \lambda_3 r(\underset{\sim}{\Theta},\underset{\sim}{\Phi}) - \lambda_4 \sum_{i=1}^{n} G_i\dot{\Theta}_i \qquad \text{(V.8)}$$

$$r_2 = [\nu_1(\underset{\sim}{\Gamma}) \sum_{i=1}^{n} G_i'\Gamma_i]' - \nu_2 \sum_{i=1}^{n} G_i'\Gamma_i + \nu_3(\underset{\sim}{\Gamma}) \sum_{i=1}^{n} G_i(\Theta_i - \Gamma_i)$$

$$- \nu_4(\underset{\sim}{\Gamma}) \sum_{i=1}^{n} G_i\dot{\Gamma}_i \qquad \text{(V.9)}$$

$$r_3 = [\omega_1(\underset{\sim}{\Gamma}) \sum_{i=1}^{n} G_i'\Phi_i]' - \omega_2(\Gamma) \sum_{i=1}^{n} G_i'\Phi_i - \omega_3(\Gamma) \sum_{i=1}^{n} G_i\Gamma_i G_i\Phi_i$$

$$- \omega_4 r(\underset{\sim}{\Theta},\underset{\sim}{\Phi}) - \omega_5 \sum_{i=1}^{n} G_i\dot{\Phi}_i \qquad \text{(V.10)}$$

where the coefficients multiplying the response variables are themselves functions of the response variables, and thus the equations are nonlinear. In accordance with the Galerkin method, the final system of ordinary differential equations was obtained by setting each residual, r_j, orthogonal to each basis function, G_i, that is

$$\int_0^1 G_i r_j d\eta = 0 \quad \begin{matrix} i = 1,2,\ldots,n; \\ j = 1,2,\ldots,n \end{matrix} \qquad \text{(V.11)}$$

The 3n ordinary differential equations given by equations V.11 retain the character of the original set of partial differential equations. Thus linear field equations transform to matrix operators and nonlinear, coupled field operators become nonlinear, coupled algebraic operators. Incorporation of the boundary conditions resulted in 3n nonlinear, coupled ordinary differential equations

$$\underset{\sim}{A}(t)\ \underset{\sim}{\Psi}(\Theta,\Gamma,\Phi) + \underset{\sim}{F}(t) = \underset{\sim}{B}(t)\ \dot{\underset{\sim}{\Psi}} \qquad \text{(V.12)}$$

subject to initial conditions, where $\underset{\sim}{B}$ is a $3n \times 3n$ matrix, $\underset{\sim}{A}$ is the operator associated with the field operator Λ_i in expression V.7, and $\underset{\sim}{F}(t)$ is an excitation vector.

Adopting the convention,

$$\langle G_i \rangle \{\Psi_i\} = \sum_{i=1}^{n} G_i \Psi_i$$

and applying the operation of expression V.11 with an integration by parts on the second order derivatives gives,

$$\{G_i\}\lambda_1\langle G_i\rangle'\{\theta\}\Big|_0^1 - \bar{\lambda}_1 \int_0^1 \{G_i\}'\langle G_j\rangle' d\eta\{\theta\}$$

$$- \bar{\lambda}_2 \int_0^1 \{G_i\}\langle G_j\rangle d\eta\{\theta\} + \bar{\lambda}_2 \int_0^1 \{G_i\}\langle G_j\rangle d\eta\{\Gamma\} \qquad \text{(V.13)}$$

$$+ \bar{\lambda}_3 \int_0^1 \{G_i\} d\eta r(\underset{\sim}{\theta},\underset{\sim}{\phi}) = \bar{\lambda}_4 \int_0^1 \{G_i\}\langle G_j\rangle d\eta\{\dot{\theta}\}$$

$$\{G_i\}\nu_1\langle G_j\rangle'\{\Gamma\}\Big|_0^1 - \bar{\nu}_1 \int_0^1 \{G_i\}'\langle G_j\rangle' d\eta\{\Gamma\}$$

$$- \bar{\nu}_2 \int_0^1 \{G_i\}\langle G_j\rangle' d\eta\{\Gamma\} + \bar{\nu}_3 \int_0^1 \{G_i\}\langle G_j\rangle d\eta\{\theta\} \qquad \text{(V.14)}$$

$$- \bar{\nu}_3 \int_0^1 \{G_i\}\langle G_j\rangle d\eta\{\Gamma\} = \bar{\nu}_4 \int_0^1 \{G_i\}\langle G_j\rangle d\nu\{\dot{\Gamma}\}$$

$$\{G_i\}\omega_1\langle G_j\rangle'\{\phi\}\Big|_0^1 - \bar{\omega}_1 \int_0^1 \{G_i\}'\langle G_j\rangle' d\eta\{\phi\}$$

$$- \bar{\omega}_2 \int_0^1 \{G_i\}\langle G_j\rangle' d\eta\{\phi\} - \bar{\omega}_3 \int_0^1 \{G_i\}\langle G_j\rangle'\{\Gamma\}\langle G_j\rangle d\eta\{\phi\}$$

$$- \bar{\omega}_4 \int_0^1 \{G_i\} d\eta r(\underset{\sim}{\theta}, \underset{\sim}{\phi}) = \bar{\omega}_5 \int_0^1 \{G_i\}\langle G_j\rangle d\eta\{\dot{\phi}\} \qquad \text{(V.15)}$$

The first term in each of the above expressions is a boundary term which permits the incorporation of natural boundary conditions which will be shown in Section V.B. Coefficients $\bar{\lambda}$, $\bar{\nu}$, $\bar{\omega}$ are variable-dependent properties, and were taken as the average value of the properties over an element. In the limit, as the elements get smaller (i.e., $n \to \infty$), the average values converge to the exact values.

Inspection of expression V.13, V.14, V.15 shows the five operators,

$$\int_0^1 \{G_i\}'\langle G_j\rangle' d\eta \qquad \text{(V.16)}$$

$$\int_0^1 \{G_i\}\langle G_j\rangle' d\eta \qquad \text{(V.17)}$$

$$\int_0^1 \{G_i\}\langle G_j\rangle d\eta \tag{V.18}$$

$$\int_0^1 \{G_i\}\langle G_j\rangle'\{\Psi\}\langle G_j\rangle d\eta \tag{V.19}$$

$$\int_0^1 \{G_i\} d\eta \tag{V.20}$$

To formulate these operators, the global shape function, G_i, was defined on the local level by

$$G_i = g_1^{(i-1)} \oplus g_2^{(i)} \tag{V.21}$$

where g_1 and g_2 were defined by

$$g_1^{(e)} = \begin{cases} (1 - \frac{\xi}{\ell_e}) & \text{for } \xi \text{ in element (e)} \\ 0 & \text{for } \xi \text{ not in element (e)} \end{cases}$$

$$g_2^{(e)} = \begin{cases} \frac{\xi}{\ell_e} & \text{for } \xi \text{ in element (e)} \\ 0 & \text{for } \xi \text{ not in element (e)} \end{cases}$$

and ℓ_e is the length of the eth element. The $\oplus$ notation in expression V.21 means that G_i is the union of $g_1^{(i-1)}$ and $g_2^{(i)}$. The local (element) shape functions have the following properties,

$$\text{(i)} \quad \int_0^{\ell_e} g_i^{(j)} \, g_k^{(m)} = 0 \quad \text{if} \quad j \neq m$$

$$\text{(ii)} \quad g_i^{(e)}(\eta_j) = \delta_{ij} = \begin{cases} 1 & \text{if} \quad i = j \\ 0 & \text{if} \quad i \neq j \end{cases}$$

Having defined the local shape functions, the elemental matrix operators contributing to the global matrix operators V.16 through V.20 are,

$$\int_0^1 \{G_i\}' \langle G_j \rangle' d\eta \quad \Rightarrow \quad \frac{1}{\ell_e} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \qquad \text{(V.16')}$$

$$\int_0^1 \{G_i\} \langle G_j \rangle' d\eta \quad \Rightarrow \quad \frac{1}{2} \begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix} \qquad \text{(V.17')}$$

$$\int_0^1 \{G_i\}\langle G_j\rangle d\eta \quad \blacklozenge \quad \frac{\ell_e}{6}\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \tag{V.18'}$$

$$\int_0^1 \{G_i\}\langle G_j\rangle'\{\Psi\}\langle G_j\rangle d\eta \quad \blacklozenge \quad \frac{-1}{3}\begin{bmatrix} (\Psi_{i-1}-\Psi_i)\left(\frac{\Psi_{i-1}-\Psi_i}{2}\right) \\ \left(\frac{\Psi_{i-1}-\Psi_i}{2}\right)(\Psi_{i-1}-\Psi_i) \end{bmatrix} \tag{V.19'}$$

$$\int_0^1 \{G_i\} d\eta \quad \blacklozenge \quad \frac{\ell_e}{2}\begin{Bmatrix} 1 \\ 1 \end{Bmatrix} \tag{V.20'}$$

The derivations of these operators are shown in Appendix E.

Since there is extensive coupling in the field equations and there are three degrees of freedom at each nodal point, the numbering scheme for the system matrices was important. To minimize the bandwidth of the matrices, the numbering scheme represented in Figure 8 was used.

Figure 9 represents the matrix $\underset{\sim}{A}(t)$ of expression V.12 for any three successive nodal points. The distribution of the elemental matrices for the FEM operators is shown, as well as the possible locations for the coupling of the field equations over an element. In addition, Figure 9 shows the bandwidth that would be observed for any n-1 element solution. For this scheme, the bandwidth is nine. If coupling is not present, the bandwidth is seven. Figure 9 reflects the extensive coupling that is present in the model. All the

matrix elemental locations are filled except those which are shaded in.

B. IMPLEMENTATION OF BOUNDARY CONDITIONS

Having formulated the system matrices for the field equations, treatment of the boundary conditions will now be discussed. Each field equation is considered individually.

1. Fiber Heat Transfer Equation

The fiber heat transfer boundary conditions in non-dimensional form from Appendix A are

$$\eta = 0 \qquad \lambda_1 \frac{\partial \Theta}{\partial \eta} = h_1 L(\Theta - 1) + \frac{\sigma \varepsilon L}{T_\infty}(\hat{T}_g^4 - \hat{T}_\infty^4) \tag{V.22}$$

$$\eta = 1 \qquad \lambda_1 \frac{\partial \Theta}{\partial \eta} = -h_2 L(\Theta - 1) - \frac{\sigma \varepsilon L}{T_\infty}(\hat{T}_g^4 - \hat{T}_\infty^4) \tag{V.23}$$

Since the first term in expression V.13 is

$$\{G_i\}\lambda_1 \langle G_j \rangle' \{\Theta\} \Big|_0^1$$

or in analogous form

$$\lambda_1 \frac{\partial \Theta}{\partial \eta} \Big|_0^1 \tag{V.24}$$

natural boundary conditions V.22 and V.23 may be directly substituted in equation V.24.

The response dependent parameters, h_1, h_2, $\hat{T}_g$, changing with time, are evaluated at the previous time step. Thus, the boundary conditions are incorporated in the system matrices as follows,

(1) $-h_1 L$: added to the stiffness matrix $\underset{\sim}{A}(t)$ at location $A_{1,1}$

(2) $h_1 L - \frac{\sigma \varepsilon L}{T_\infty}(\hat{T}_g^4 - \hat{T}_\infty^4)$: added to the excitation vector $\underset{\sim}{F}(t)$ at location F_1

(3) $-h_2 L$: added to the stiffness matrix $\underset{\sim}{A}(t)$ at location $A_{3n-2,3n-2}$

(4) $h_2 L - \frac{\sigma \varepsilon L}{T_\infty}(\hat{T}_g^4 - \hat{T}_\infty^4)$: added to the excitation vector $\underset{\sim}{F}(t)$ at location F_{3n-2}

2. Internal Flow Heat Transfer Equation

The non-dimensional boundary conditions presented in Appendix A for the air energy equation are

$$\eta = 0 \qquad \Gamma = 1 \tag{V.25}$$

$$\eta = 1 \qquad \frac{\partial \Gamma}{\partial \eta} = \frac{\partial \Theta}{\partial \eta} \tag{V.26}$$

The essential boundary condition at $\eta = 0$, $\Gamma(\eta = 0) = 1$ is imposed in the Galerkin equation as follows. The $A_{2,i}$ row of the $\underset{\sim}{A}(t)$ matrix, the $B_{2,i}$ row and the $B_{i,2}$ column of the $\underset{\sim}{B}$ matrix, and the F_2 location of the excitation vector, $\underset{\sim}{F}(t)$,

are all set equal to zero. The $B_{2,2}$ location of the $\underset{\sim}{B}$ matrix is then set equal to one. The natural boundary condition at $\eta = 1$ for the air heat transfer equation was treated in the same manner as that of the fiber heat transfer equation. Foregoing the individual steps the boundary condition is implemented by

(1) $-\frac{h_2 L \nu_1}{\lambda_1}$: added to the stiffness matrix $\underset{\sim}{A}(t)$ at location $A_{3n-1,3n-2}$

(2) $\frac{h_2 L \nu_1}{\lambda_1} - \frac{\sigma \varepsilon \nu_1}{T_\infty \lambda_1}(\hat{T}_g^4 - \hat{T}_\infty^4)$: added to the excitation vector $\underset{\sim}{F}(t)$ at location F_2.

3. Oxygen Transport Equation

For the oxygen diffusion equation, the boundary conditions in non-dimensional form from Appendix A are:

$$\eta = 0 \qquad \omega_1 \frac{\partial \phi}{\partial \eta} = \omega_2(\phi - p) \qquad \text{(V.27)}$$

$$\eta = 1 \qquad \frac{\partial \phi}{\partial \eta} = 0 \qquad \text{(V.28)}$$

Since these are both natural boundary conditions, they were substituted for the first term in expression V.15 at $\eta = 0$ and $\eta = 1$, respectively. Coefficients ω_1 and ω_2 are evaluated at the previous time step. The boundary conditions are implemented by adding

(1) $-\omega_2$: to the stiffness matrix $\underset{\sim}{A}(t)$ at location $A_{3,3}$

and

(2) $\omega_2 p$: to the excitation vector $\underset{\sim}{F}(t)$ at location F_3

This concludes the discussion for the implementation of the boundary conditions. A word of caution is in order. After each time step integration, the time-dependent coefficients of the boundary conditions (i.e., h_1, h_2, λ, ν, ω) are reevaluated. Before incorporating the updated coefficients into the stiffness matrix $\underset{\sim}{A}(t)$, the previous values must be subtracted out. The results of not taking this into account will be obvious.

The implicit system of ordinary differential equations was integrated numerically by a modified implicit-Gear method developed by Franke [2]. The time-dependent coefficients of the FEM operators in expression V.13, V.14, and V.15 were updated at the previous time. The reaction rate term (III.26) was also evaluated at the previous time, and appears in the excitation vector $\underset{\sim}{F}(t)$. In this way, the final system of ordinary differential equations was

$$\underset{\sim}{A}(t)\underset{\sim}{\Psi} + \underset{\sim}{F}(t) = \underset{\sim}{B}\dot{\underset{\sim}{\Psi}}$$

where $\underset{\sim}{A}$ and $\underset{\sim}{B}$ are $(3n \times 3n)$ matrices of temperature dependent

coefficients. $\underset{\sim}{F}$ is a $(3n \times 1)$ vector arising partly from the reaction rate terms and partly from the boundary conditions. As noted, the elements of $\underset{\sim}{F}$ are dependent on both temperature and oxygen concentration.

VI. RESULTS AND CONCLUSION

A. NUMERICAL CONSIDERATIONS

The input parameters which were varied in the computer analysis include (1) plate thickness, L, (2) fiber diameter, d, and (3) air flow rate, U_∞. Other parameters which could be varied are the ply thickness, D, ambient temperature, T_∞, and fiber emissivity, ϵ. One set of initial conditions was used for the analysis. These are shown in Figures 10 and 11. For this initial effort, the actual initial conditions were not of prime consideration. The selection of initial conditions of Figures 10 and 11 will be discussed in Section VI.C. The finite element program calculates the remaining system parameters such as permeability, porosity, pressure differential, and the response variables as functions of time and position. Parameters which are functions of temperature, such as k_a, k_g, k_r, h_i, ρ_a, u_p, and μ are continuously updated during the transient analysis.

The preliminary solution effort showed the system of equations to be very stiff (refer to Shampine/Gordon [24] and Gear [25] for a discussion of "stiffness"). Changing the integration algorithm from a sixth-order Runge-Kutta (IMSL subroutine DVERK) to a modified implicit-Gear method for stiff systems, developed by Franke [2], resulted in a significant reduction in CPU time. The computational effort

was carried out on an IBM 360/70. Typical runs required 20-30 minutes CPU time for problems for which ignition occurred, and 6-25 minutes CPU time for extinction problems. Ignition problems were terminated when the temperature at any nodal point exceeded 2200 degrees Fahrenheit, or when the graphite at a nodal point was totally consumed. Extinction problems were carried out to steady state.

A twenty five nodal point model (75 o. d. e.) provided results which differed less than five percent from the results of a 32 nodal point model (96 o. d. e.) and was adopted for all computer runs. For the twenty five nodal point model, approximately 275K bytes of core was required. The computer program which includes the FEM formulation and the integration routine as well as a sample input file is presented at the end of the appendices.

The numerical solution produced satisfactory results with one exception which will now be discussed. For a particular range of temperature and oxygen concentration (approximately 1500 degrees Fahrenheit and .001 lbm/ft^3, respectively), there is a significant increase in reaction rate. This accelerated reaction rate produced a negative/positive oscillation for the nodal values of oxygen concentration. The oscillation occurred in a region of the plate where the oxygen appeared to be totally consumed. As discussed by Frank-Kamenetskii [3], nth order reactions may yield zero values for the oxygen concentration and gradient within the

medium. The cause of the oscillation was as follows. Although the reaction rate is a function of temperature and oxygen concentration, numerically, it is treated as constant during an integration interval. As a result, the concentration in the region of high reaction rate becomes negative. The reaction rate was updated for the next time interval by setting negative concentrations to zero. During this time interval, for the region of zero concentration, there is no reaction. Without consumption, the oxygen concentration will increase and the cycle repeats itself. The oscillation was aggravated by large plate thickness and low permeability. The instability occurring for the high reaction rate may be corrected by (1) numerically integrating the rate term in the time domain, (2) iterating until convergence is obtained between consecutive values of concentration, or (3) decreasing the time step and the length of the elements. As a matter of expediency, measure (3) was used to minimize the instability. The fiber and air temperatures were essentially unaffected by the oscillations in the oxygen concentration.

B. RESULTS AND OBSERVATIONS

Table 1 presents the results of fourteen problems. In Table 1, the parameters which depend upon temperature (u_p, Re_i, and h_i) are evaluated at ambient conditions for comparison purposes only. These parameters, in fact, will vary during the course of the transient analysis. In all cases,

the initial condition on graphite temperature was 1050 degrees Fahrenheit.

Figures 10, 11, and 12 show the transient behavior of Case 1. For the initial conditions shown, ignition occurred in approximately eight seconds. The reaction rate and oxygen concentration responses for Case 1 are typical of the problems for which ignition resulted. Figure 13 shows that the air and fiber temperatures for Case 1 do not differ significantly. This behavior is typical for most problems. However, for plates with high porosity (greater than .8) and subjected to relatively high flow rates, significant differences in the air and fiber temperatures do occur (see Figure 14 for Case 9). In a previous effort by Vatikiotis and Salinas [26], linearly varying initial conditions were investigated. Although the reaction rate used in that investigation differed from the one used in the present investigation, the overall results remain valid. The main observation was that ignition is less likely to occur for thin plates with the ambient air entering the hotter plate surface. Since temperature controls the reaction in the kinetic regime, cooler air entering the hotter plate surface enhances the heat loss. This reduces the fiber temperature, thereby decreasing the reaction rate. In effect, the cooler air enters the plate where it is most needed.

In the present analysis, observations were made by varying one input parameter (i.e., L or d or U_∞) while keeping

all others fixed. The effects of each parameter on the behavior will be discussed individually.

1. Effects of Exterior Velocity

As shown in Figures 15, 16 and 17 (cases 4, 1 and 2, respectively) for an initial condition of 1050 degrees Fahrenheit, three distinct regions of combustion were observed (extinction-ignition-extinction). These became apparent as U_∞ was increased from low velocities (10 knots) to higher velocities (120 knots). Vulis [4] discusses an experiment of a heated carbon rod with an air jet impinging upon it. For a certain range of flow velocities, ignition was observed. However, extinction did occur for velocities less than and greater than the velocity for which ignition occurred. The behavior of the carbon rod and that of the graphite mat is similar. This behavior may be explained by the Semenov model of Figure 1. For high U_∞, the internal heat transfer coefficient, h_i, will be large as a result of an increase in the pore velocity. Since the slopes of the heat loss lines, q_ℓ, increase with increasing h_i for a constant T_a, the graphite temperature decreases from the critical ignition point I. This causes extinction for the higher exterior flow velocities, U_∞. In contrast, for low U_∞, the slope of q_ℓ will be small and ignition is more likely to occur. However, the heat generation curve, q_g, changes position due to a decrease in oxygen concentration. This reduction in oxygen concentration is caused by the lower induced flow rate through the

plate. The overall shape of q_g is flattened such that the q_ℓ line crosses q_g behind the new critical point I. Thus extinction is observed for this region of low U_∞.

2. Effects of Fiber Diameter

Varying the fiber diameter with the remaining input parameters fixed, also yields three regions of combustion (extinction-ignition-extinction) for a fixed initial temperature. The results are shown in Figures 16, 18 and 19 (Cases 1, 9 and 10, respectively). The fiber diameter and ply thickness determine the permeability of the plate. Similar to U_∞, permeability affects the pore velocity (i.e., low permeability → low velocity). In turn, this affects the convective heat transfer and the amount of oxygen entering the plate. These three regions of combustion are explained by the Semenov model for the same reasons as those of varying U_∞.

Porosity is a measure of void space and denotes the space available for oxygen. Porosity is associated with the internal geometry of the medium, as is permeability. However, they are basically different parameters. Permeability (hydraulic conductivity) is associated with convective air flow through the medium. Thus, an n-fold increase in the fiber diameter and ply thickness will not affect a change in porosity, but will affect an n^2 order change in the permeability. For an n greater than one, the result is a decrease in pore velocity without a change in porosity. Porosity

determines the maximum oxygen concentration per unit volume of fibrous mat. This indirectly affects the reaction rate. Thus, for a given u_p, the lower the porosity, the less oxygen there is for combustion. It appears that high porosity would enhance combustion by the presence of more oxygen. However, higher porosities also provide more fluid per unit volume resulting in greater heat transfer. This is observed in Case 9, Figure 18.

3. Effects of Plate Thickness, L

For the given initial temperature of 1050 degrees Fahrenheit, varying the plate thickness yielded two regions of combustion (extinction-ignition). Extinction was observed for thin plates (Case 2, Figure 17). As shown by Figures 20 and 21 (Cases 7 and 11, respectively), ignition was observed when plate thickness was increased. Plate thickness also affects the pore velocity. Decreasing L, increases the pressure gradient across the plate, thus increasing the pore velocity. The result is that extinction is more likely for thin plates because of the enhanced convection heat transfer resulting from the increase in pore velocity. Whereas pore velocity is inversely proportional to L, it is an exponential function of U_∞. For the range of parameters in this investigation (i.e., .1" < L < 3.", and 10 knots < U_∞ < 100 knots), an n-fold change in U_∞ will produce a greater change in u_p, then will an n-fold change in L. Compare Cases 1 and 2 to Cases 7 and 8.

A characteristic feature of ignition for thick plates was observed. As the thickness increased, the ignition region (the spatial location) moved closer to the entrance surface of the ambient air. Compare Figures 20 and 21.

C. DISCUSSION

At this point, discussion is made of ignition temperatures for porous graphite plates. The ignition temperature for Case 1 was 1050 degrees Fahreheit. This temperature was obtained by varying the initial temperature until ignition occurred. In all subsequent cases, 1050 degrees Fahrenheit was adopted as the initial condition, and we observed whether extinction or ignition occurred. The ignition temperatures given here are the result of taking $n = \frac{1}{2}$ in the nth order reaction rate. Significantly different ignition temperatures will result for other n. For example, for n = 1 (1st order reaction), the ignition temperature for Case 1 was approximately 1600 degrees Fahrenheit. As Frank-Kamenetskii [3] has suggested values of n between 1/3 and 2/3, the average value of 1/2 was adopted for this analysis. The ignition temperatures obtained using $n = \frac{1}{2}$ agree favorably with the experiments of Fontenot [1]. For fiber combustion, ignition temperatures for porous graphite plates are on the order of 1100 degrees Fahrenheit.

Consider the results of varying U_∞. Extinction occurred for Case 2 and Case 4; thus, the ignition temperature

for each case is greater than 1050 degrees Fahrenheit. Since ignition does occur at 1050 degrees Fahrenheit for intermediate values of U_∞ (Case 1, Case 7), ignition temperature is not a monotonic function of U_∞. The precise determination of ignition temperature for a specific value of air velocity can be obtained by a large number of computer runs. A similar discussion can be made for the ignition temperatures dependence on fiber diameter. The general shape of these functions is represented by the shaded region on Figure 22. These suppositions may only be valid in the limited range of parameters associated with the present investigation.

It is interesting to observe that changing the initial condition of the oxygen concentration only affects the early part of the problem. The response of the concentration is fast compared to that of temperature. After approximately one second, the transient behavior is the same regardless of the initial condition on the oxygen concentration.

A brief description of the Semenov model was given in Section II.A. That discussion was for a lumped parameter model. The actual combustion process is more complex since there are spatial variations in temperature and in oxygen concentration. The results of this analysis show that both kinetic and diffusion regimes may exist simultaneously in a porous medium. Hence, it is not reasonable to restrict an

analysis of combustion in a porous medium to the kinetic regime.

D. CONCLUDING REMARKS

The model has provided considerable insight as to the behavior of fibrous composites subject to combustion. Improvements may be realized by extending the model to include:

(1) The combustion of the epoxy matrix (i.e., start problem with first stage of combustion process).

(2) The change in geometry of the porous medium due to combustion (affects p, m and z).

(3) A more complex reaction (i.e., secondary combustion of gaseous by-products, such as carbon monoxide).

(4) The effect of gaseous by-products on fluid properties.

(5) Generalization to two and three dimensional models (results in anisotropic properties).

The results show that certain properties, such as plate thickness, permeability and porosity, have significant effects on combustion. Therefore, one could select these design parameters to improve the flame resistance of composite materials. This would be beneficial to the survivability of a composite structure. A comprehensive set of analyses could be undertaken to couple the combustion problem to the strength problem. In this way, one could achieve a design which maximizes strength and minimizes combustion.

Another use of the present model would be in the study of energy systems utilizing particulate fuels (i.e., coal, biomass). In this case, the design parameters could be selected to maximize the performance of the system.

APPENDIX A

NONDIMENSIONALIZATION OF FIELD EQUATIONS

The field equations and boundary conditions are:

$$\frac{\partial}{\partial x}[(k_g+k_r)\frac{\partial T_g}{\partial x}] - \frac{h_i z}{(1-p)}(T_g-T_a) + \Delta Hr(T_g,\phi) = \rho_g c_g \frac{\partial T_g}{\partial t} \qquad \text{(III.28)}$$

$$\frac{\partial}{\partial x}(k_a \frac{\partial T_a}{\partial x}) - \dot{m} c_a \frac{\partial T_a}{\partial x} + \frac{h_i z}{p}(T_g-T_a) = \rho_a c_a \frac{\partial T_a}{\partial t} \qquad \text{(III.37)}$$

$$\frac{\partial}{\partial x}(B\frac{\partial \phi}{\partial x}) - u_p \frac{\partial \phi}{\partial x} - \frac{\partial u_p}{\partial T_a}(\frac{\partial T_a}{\partial x})\phi - (\frac{1}{f})r(T_g,\phi) = \frac{\partial \phi}{\partial t} \qquad \text{(III.46)}$$

<u>at x = 0</u>

$$(k_g+k_r)\frac{\partial T_g}{\partial x} = h_1(T_g-T_\infty) + \sigma\varepsilon(\hat{T}_g^4-\hat{T}_\infty^4) \qquad \text{(IV.1)}$$

$$T_a = T_\infty \qquad \text{(IV.3)}$$

$$B\frac{\partial \phi}{\partial x} = u_p(\phi - p\phi_\infty) \qquad \text{(IV.5)}$$

<u>at x = L</u>

$$(k_g+k_r)\frac{\partial T_g}{\partial x} = -h_2(T_g-T_\infty) - \sigma\varepsilon(\hat{T}_g^4-\hat{T}_\infty^4) \qquad \text{(IV.2)}$$

$$\frac{\partial T_a}{\partial x} = \frac{\partial T_g}{\partial x} \qquad \text{(IV.4)}$$

$$\frac{\partial \phi}{\partial x} = 0 \qquad \text{(IV.6)}$$

The nondimensional variables are defined as:

$\Theta = T_g/T_\infty$ nondimensional fiber temperature

$\Gamma = T_a/T_\infty$ nondimensional air temperature

$\Phi = \phi/\phi_\infty$ nondimensional oxygen concentration

$\eta = x/L$ nondimensional distance

The time variable, t, will not be nondimensionalized.

Using the temperature of the fiber, T_g, to demonstrate the technique of transformation, we have,

$$T_g = T_\infty \Theta$$

It follows that,

$$\frac{\partial T_g}{\partial x} = T_\infty \frac{\partial \Theta}{\partial x}$$

$$\frac{\partial^2 T_g}{\partial x^2} = T_\infty \frac{\partial^2 \Theta}{\partial x^2}$$

Using the chain rule to transform x to η, gives

$$\frac{\partial T_g}{\partial x} = T_\infty \frac{\partial \Theta}{\partial \eta} \frac{\partial \eta}{\partial x}$$

Since $\eta = x/L$, the partial derivatives become

$$\frac{\partial T_g}{\partial x} = \frac{T_\infty}{L}\frac{\partial \Theta}{\partial \eta}$$

and

$$\frac{\partial^2 T_g}{\partial x^2} = \frac{T_\infty}{L}\frac{\partial^2 \Theta}{\partial \eta^2}\frac{\partial \eta}{\partial x}$$

Therefore,

$$\frac{\partial^2 T_g}{\partial x^2} = \frac{T_\infty}{L^2}\frac{\partial^2 \Theta}{\partial \eta^2}$$

Similar transformations for T_a and ϕ yield,

$$\frac{\partial T_a}{\partial x} = \frac{T_\infty}{L}\frac{\partial \Gamma}{\partial \eta} \qquad \frac{\partial \phi}{\partial x} = \frac{\phi_\infty}{L}\frac{\partial \phi}{\partial \eta}$$

$$\frac{\partial^2 T_a}{\partial x^2} = \frac{T_\infty}{L^2}\frac{\partial \Gamma}{\partial \eta} \qquad \frac{\partial^2 \phi}{\partial x^2} = \frac{\phi_\infty}{L^2}\frac{\partial^2 \phi}{\partial \eta^2}$$

Substituting these relations into the field equations and removing the constants from the differential operators gives,

$$\frac{T_\infty}{L^2}\frac{\partial}{\partial \eta}\left[(k_g+k_r)\frac{\partial \Theta}{\partial \eta}\right] - \frac{h_i z}{(1-p)}(\Theta-\Gamma) + \Delta Hr(T_g,\phi) = \rho_g c_g \frac{\partial \Theta}{\partial t}$$

$$\frac{T_\infty}{L^2}\frac{\partial}{\partial \eta}\left(k_a\frac{\partial \Gamma}{\partial \eta}\right) - \frac{\dot{m}c_a T_\infty}{L}\frac{\partial \Gamma}{\partial \eta} + \frac{h_i z}{p}(\Theta-\Gamma) = \rho_a c_a \frac{\partial \Gamma}{\partial t}$$

$$\frac{\phi_\infty}{L^2}\frac{\partial}{\partial\eta}(B\frac{\partial\phi}{\partial\eta}) - \frac{u_p T_\infty}{L}\frac{\partial\phi}{\partial\eta} - \frac{\phi_\infty T_\infty}{L}(\frac{\partial u_p}{\partial T_a})\frac{\partial\Gamma}{\partial\eta}\phi - (\frac{1}{f})r(T_g,\phi) = \phi_\infty\frac{\partial\phi}{\partial t}$$

Upon rearrangement, the equations become,

$$\frac{\partial}{\partial\eta}[(k_g+k_r)\frac{\partial\Theta}{\partial\eta}] - \frac{h_i z L^2}{(1-p)}(\Theta-\Gamma) + \frac{\Delta H L^2}{T_\infty}r(T_g,\phi) = \rho_g c_g L^2\frac{\partial\Theta}{\partial t}$$

$$\frac{\partial}{\partial\eta}(k_a\frac{\partial\Gamma}{\partial\eta}) - \dot{m}c_a L\frac{\partial\Gamma}{\partial\eta} + \frac{h_i z L^2}{p}(\Theta-\Gamma) = \rho_a c_a L^2\frac{\partial\Gamma}{\partial t}$$

$$\frac{\partial}{\partial\eta}(B\frac{\partial\phi}{\partial\eta}) - u_p L\frac{\partial\phi}{\partial\eta} - T_\infty L(\frac{\partial u_p}{\partial T_a})\frac{\partial\Gamma}{\partial\eta}\phi - (\frac{1}{f})\frac{L^2}{\phi_\infty}r(T_g,\phi) = L^2\frac{\partial\phi}{\partial t}$$

Letting,

$$\lambda_1 = (k_g+k_r) \qquad \lambda_2 = \frac{h_i z L^2}{(1-p)} \qquad \lambda_3 = \frac{\Delta H L^2}{T_\infty} \qquad \lambda_4 = \rho_g c_g L^2$$

$$\nu_1 = k_a \qquad \nu_2 = \dot{m}c_a L \qquad \nu_3 = \frac{h_i z L^2}{P} \qquad \nu_4 = \rho_a c_a L^2$$

$$\omega_1 = B \qquad \omega_2 = u_p L \qquad \omega_3 = T_\infty L\frac{\partial u_p}{\partial T_a} \qquad \omega_4 = \frac{1}{f}\frac{L^2}{\phi_\infty}$$

$$\omega_5 = L^2$$

the field equations may be written as,

$$\frac{\partial}{\partial\eta}(\lambda_1\frac{\partial\Theta}{\partial\eta}) - \lambda_2(\Theta-\Gamma) + \lambda_3 r(T_g,\phi) = \lambda_4\frac{\partial\Theta}{\partial t} \qquad \text{(A.1)}$$

$$\frac{\partial}{\partial\eta}(\nu_1\frac{\partial\Gamma}{\partial\eta}) - \nu_2\frac{\partial\Gamma}{\partial\eta} + \nu_3(\Theta-\Gamma) = \nu_4\frac{\partial\Gamma}{\partial t} \qquad \text{(A.2)}$$

$$\frac{\partial}{\partial \eta}(\omega_1 \frac{\partial \phi}{\partial \eta}) - \omega_2 \frac{\partial \phi}{\partial \eta} - \omega_3 \frac{\partial \Gamma}{\partial \eta}\phi - \omega_4 r(T_g, \phi) = \omega_5 \frac{\partial \phi}{\partial t} \quad (A.3)$$

Noting that the coefficients λ, ν, ω are response dependent variables, equations A.1, A.2, and A.3 are considered in their final form in Section III.

Substituting the nondimensional variables into the boundary conditions gives,

$$\lambda_1 \frac{\partial \Theta}{\partial \eta} = h_1 L(\Theta - 1) + \frac{\sigma \varepsilon L}{T_\infty}(\hat{T}_g^4 - \hat{T}_\infty^4) \qquad x = 0$$

$$\Gamma = 1 \qquad x = 0$$

$$\omega_1 \frac{\partial \Phi}{\partial \eta} = \omega_2(\Phi - p) \qquad x = 0$$

and

$$\lambda_1 \frac{\partial \Theta}{\partial \eta} = -h_2 L(\Theta - 1) - \frac{\sigma \varepsilon L}{T_\infty}(\hat{T}_g^4 - \hat{T}_\infty^4) \qquad x = L$$

$$\frac{\partial \Gamma}{\partial \eta} = \frac{\partial \Theta}{\partial \eta} \qquad x = L$$

$$\frac{\partial \Phi}{\partial \eta} = 0 \qquad x = L$$

The dimensional form of the absolute temperature will be retained for convenience.

APPENDIX B

POLYNOMIAL APPROXIMATIONS OF THERMAL PROPERTIES

Relations giving the viscosity and thermal conductivities of air for varying temperature were required. A simple way to obtain values for these properties is to fit empirical data with 2nd order Lagrange polynomials.

The general form of the 2nd order Lagrange polynomials for thermal conductivity and viscosity are

$$k_a = \frac{(T_a-T_{a2})(T_a-T_{a3})}{(T_{a1}-T_{a2})(T_{a1}-T_{a3})} k_{a1} + \frac{(T_a-T_{a3})(T_a-T_{a1})}{(T_{a2}-T_{a3})(T_{a2}-T_{a1})} k_{a2} + \frac{(T_a-T_{a1})(T_a-T_{a2})}{(T_{a3}-T_{a1})(T_{a3}-T_{a2})} k_{a3} \qquad (B.1)$$

$$\mu = \frac{(T_a-T_{a2})(T_a-T_{a3})}{(T_{a1}-T_{a2})(T_{a1}-T_{a3})} \mu_1 + \frac{(T_a-T_{a3})(T_a-T_{a1})}{(T_{a2}-T_{a3})(T_{a2}-T_{a1})} \mu_2 + \frac{(T_a-T_{a1})(T_a-T_{a2})}{(T_{a3}-T_{a1})(T_{a3}-T_{a2})} \mu_3 \qquad (B.2)$$

Choosing three points from a range of temperatures that would be representative of those observed during the analysis, the corresponding values of the properties are:

(subscript)	Temp (F)	k_a ($\frac{\text{Btu}}{\text{lbm-hr-ft}}$)	μ ($\frac{\text{lbm}}{\text{ft-hr}}$)
1	0	.0131	.0394
2	700	.0284	.0765
3	1500	.0423	.107

Substituting these values into expressions B.1 and B.2 gives,

$$k_a = \frac{(T_a-700)(T_a-1500)}{(0-700)(0-1500)}(.0131) + \frac{(T_a-1500)(T_a-0)}{(700-1500)(700-0)}(.0284)$$

$$+ \frac{(T_a-0)(T_a-700)}{(1500-0)(1500-700)}(.0423)$$

$$\mu = \frac{(T_a-700)(T_a-1500)}{(0-700)(0-1500)}(.0394) + \frac{(T_a-1500)(T_a-0)}{(1500-0)(1500-700)}(.0765)$$

$$+ \frac{(T_a-0)(T_a-700)}{(1500-0)(1500-700)}(.107)$$

These expressions reduce to,

$$k_a = -3.232 \times 10^{-9} T_a^2 + 2.412 \times 10^{-5} T_a + .0131 \quad \frac{\text{Btu}}{\text{lbm-hr-ft}}$$

$$\mu = -1.041 \times 10^{-8} T_a^2 + 6.029 \times 10^{-5} T_a + .0394 \quad \frac{\text{lbm}}{\text{ft-hr}}$$

Both expressions give property values which are within five percent of the data for temperatures to 2000 degrees Fahrenheit.

APPENDIX C

TRANSFORMATION OF THE REACTION RATE TERM

The expression for the oxidation rate of graphite fibers taken from Parker and Hottel [15] is

$$r_g = \frac{9.55 \times 10^6}{\hat{T}_{gk}^{1/2}} P_{02} \exp\left(\frac{-44000}{R\ \hat{T}_{gk}}\right) \qquad \frac{gm}{cm^2\text{-sec}} \qquad (C.1)$$

where R is the universal gas constant (1.958 cal/gmole-K) and P_{02} is the partial pressure of oxygen (atm.). The partial pressure may be represented in terms of the temperature, $\hat{T}$, and oxygen concentration, ϕ, by the Ideal Gas law in the form given by Kanury [16]

$$P_{02} = \left(\frac{M_a}{M_{02}}\right) R_A\ \hat{T}\ \phi \qquad (C.2)$$

where $M_a/M_{02} = .9$ is the ratio of the molecular weights of air and oxygen; R_A (= 53.34 ft.-lbf/lbm R) is the gas constant for air. Substituting M_a/M_{02} into equation C.2 and converting P_{02} to atmospheric units the expression becomes

$$P_{02} = 4.25 \times 10^{-4} R_A\ \hat{T}\ \phi \quad \text{atm.}$$

Converting r_g to lbm/ft^2-hr from gm/cm^2-sec, equation C.1 becomes

$$r_g = \frac{7.04 \times 10^{10}}{T_{gk}^{1/2}} P_{02} \exp\left(\frac{-44000}{R\ T_{gk}}\right) \quad \frac{\text{lbm}}{\text{ft}^2\text{-hr}}$$

Substituting in for P_{02} and converting the absolute temperatures from Kelvin to Rankine, the rate expression becomes,

$$r_g = 4.014 \times 10^7 \frac{R_A\ \hat{T}\ \phi}{\hat{T}_g^{1/2}} \exp\left(\frac{-39883}{\hat{T}_g}\right) \quad \frac{\text{lbm}}{\text{ft}^2\text{-hr}}$$

The absolute temperature at the fiber surfaces is $\hat{T}_g$. Thus, $\hat{T}$ in the numerator becomes $\hat{T}_g$, and the expression becomes

$$r_g = 4.014 \times 10^7\ R_A\ T_g^{1/2}\ \phi \exp\left(\frac{-39883}{T_g}\right)$$

To transform the reaction rate to lbm/ft^3-hr, y, the ratio of a fibers surface area to its volume is placed in the numerator of r_g. The expression for y is,

$$y = \frac{1}{2} \frac{\pi d}{\frac{\pi}{4} d^2} = \frac{2}{d} \qquad \text{(C.3)}$$

where d is the fiber diameter, and the $\frac{1}{2}$ factor accounts for the uncertainty of the actual amount of fiber surface after the epoxy has burned away. The reaction rate of the graphite

fibers per unit volume is expressed as

$$r = 4.014 \times 10^7 \; y \; R_A \; \hat{T}_g^{1/2} \; \phi \; \exp\left(\frac{-39883}{\hat{T}_g}\right) \quad \frac{lbm}{ft^3\text{-}hr}$$

To obtain the heat liberated per lbm of fiber, r is multiplied by ΔH, the enthalpy of formation of carbon dioxide per unit mass of graphite consumed. This value is approximately 14,085 BTU per pound-mass of fiber and was obtained from Kanury [16]

$$\text{Heat generation rate} = \Delta H \; r(T_g, \phi)$$

To obtain the oxygen consumption rate, r is multiplied by the inverse of the fuel-air stoichiometric ratio,

$$\text{Oxygen consumption rate} = \left(\frac{1}{f}\right) r(T_g, \phi).$$

APPENDIX D

JUSTIFICATION OF THE DANKWERTS' BOUNDARY CONDITIONS

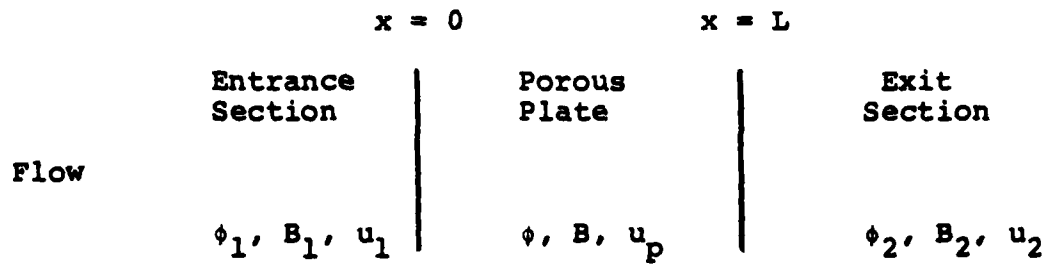
The Dankwerts' boundary conditions for the oxygen diffusion equation are:

$$\frac{d\phi}{dx} = \frac{u_p}{B}(\phi - p\phi_\infty) \qquad x = 0$$

$$\frac{d\phi}{dx} = 0 \qquad x = L$$

Bischoff [23] presents a discussion of these equations. A brief summary is provided for completeness.

Figure 10 shows the one-dimensional oxygen transport region considered in this analysis.



The concentration of oxygen, ϕ, for each region is distinguished by subscripts; B and u are the diffusivity and the velocity, respectively, for each region. The oxygen diffusion equations for each section are as follows,

$$\frac{B_1}{u_1}\frac{d^2\phi_1}{dx^2} - \frac{d\phi}{dx} = 0 \qquad x \le 0 \qquad \text{(D.1)}$$

$$\frac{B}{u_p}\frac{d^2\phi}{dx^2} - \frac{d\phi}{dx} - r(T,\phi) = 0 \qquad 0 \le x \le L \qquad \text{(D.2)}$$

$$\frac{B_2}{u_2}\frac{d^2\phi}{dx^2} - \frac{d\phi_2}{dx} = 0 \qquad x \ge L \qquad \text{(D.3)}$$

with the general boundary conditions,

$$\phi_1(-\infty) = \phi_\infty \qquad \text{(D.4)}$$

$$p\phi_1(0^-) = \phi(0^+) \qquad \text{(D.5)}$$

$$p\phi_1(0^-) - p\frac{B_1}{u_1}\frac{d\phi_1(0^-)}{dx} = \phi(0^+) - \frac{B}{u_p}\frac{d\phi(0^+)}{dx} \qquad \text{(D.6)}$$

$$p\phi(L^-) = \phi_2(L^+) \qquad \text{(D.7)}$$

$$p\phi(L^-) - p\frac{B}{u_p}\frac{d\phi(L^-)}{dx} = \phi_2(L^+) - \frac{B_2}{u_2}\frac{d\phi_2(L^+)}{dx} \qquad \text{(D.8)}$$

$$\phi_2(+\infty) = \text{finite} \qquad \text{(D.9)}$$

For convenience, the parameters u_i, B_i will be treated as constant. In addition, the porosity, p, has been included to account for the discontinuity that exist for the concentration. The discontinuity is caused by the oxygen from a totally gaseous environment to one that is partly occupied by solid.

An analytical closed-form solution for this set of equations is not possible because of the nonlinearity of equation D.2. However, the solutions of equations D.1 and D.3 are,

$$\phi_1 = A_1 + A_2 \exp(u_1 x/B_1) \qquad (D.10)$$

$$\phi_2 = A_3 + A_4 \exp(u_2 x/B_2) \qquad (D.11)$$

Applying boundary conditions D.4 and D.9, the following results are obtained,

$$A_1 = \phi_\infty$$

$$A_4 = 0$$

The solutions D.10 and D.11 become

$$\phi_1 = \phi_\infty + A_2 \exp(u_1 x/B_1) \qquad (D.12)$$

$$\phi_2 = A_3 \tag{D.13}$$

It would be necessary to have the solution for the non-linear equation D.2 to solve for A_2 and A_3. However, the constants need not be known to continue with the analysis.

From equation D.12,

$$\phi_1(0^-) = \phi_\infty + A_2$$

and,

$$\frac{d\phi_1(0^-)}{dx} = \frac{u_1}{B_1} A_2$$

Substituting these into equation D.9 gives

$$p\phi_\infty + pA_2 - p \frac{B_1}{u_1}\left(\frac{u_1}{B_1} A_2\right) = \phi(0^+) - \frac{B}{u_p} \frac{d\phi(0^+)}{dx}$$

Cancelling terms yields,

$$p\phi_\infty = \phi(0^+) - \frac{B}{u_p} \frac{d\phi(0^+)}{dx}$$

Rearranging, the Dankwerts' boundary condition at x = 0 is

$$\frac{d\phi}{dx} = \frac{u_p}{B}(\phi - p\phi_\infty) \qquad x = 0$$

From equation D.13, and noting that A_3 is a constant, we have

$$\frac{d\phi_2}{dx} = 0$$

and

$$\frac{d\phi_2(L^+)}{dx} = 0$$

Substituting these expressions and equation D.7 into equation D.8,

$$p\phi(L^-) - p\frac{B}{u_p}\frac{d\phi(L^-)}{dx} = p\phi(L^-) - \frac{B_2}{u_2}(0)$$

Upon cancelling terms, the second Dankwets' boundary condition becomes,

$$\frac{d\phi}{dx} = 0 \qquad\qquad x = L$$

An important underlying consideration for using the Dankwerts' boundary conditions is that it simplifies the analysis since equation D.2 may be solved independently without haveing to consider entrance and exit regions.

APPENDIX E

DERIVATION OF THE FEM OPERATORS

In the section on the finite element formulation, the following five differential operators were identified,

$$\int_0^1 \{G_i'\}\langle G_j'\rangle d\eta \tag{E.1}$$

$$\int_0^1 \{G_i\}\langle G_j'\rangle d\eta \tag{E.2}$$

$$\int_0^1 \{G_i\}\langle G_j\rangle d\eta \tag{E.3}$$

$$\int_0^1 \{G_i\}\langle G_j'\rangle\{\Psi\}\langle G_j\rangle d\eta \tag{E.4}$$

$$\int_0^1 \{G_i\} d\eta \tag{E.5}$$

where the G_i are the global basis functions. These operators are constructed on the element level by introducing the corresponding element basis functions, g_i. The global and element basis functions are related by,

$$G_i = g_1^{(i-1)} \oplus g_2^{(i)}$$

where g_1 and g_2 are defined by

$$g_1^{(e)} = \begin{cases} (1 - \frac{\xi}{\ell_e}) & \text{for } \xi \text{ in element (e)} \\ 0 & \text{for } \xi \text{ not in element (e)} \end{cases}$$

$$g_2^{(e)} = \begin{cases} \frac{\xi}{\ell_e} & \text{for } \xi \text{ in element (e)} \\ 0 & \text{for } \xi \text{ not in element (e)} \end{cases}$$

and ℓ_e is the length of the (e)th element.

The derivation of the local elemental matrices according to the Galerkin method for the global operations E.1 through E.5 proceeds as follows:

For operator E.1,

<u>global</u>		<u>local</u>
$\int_0^1 \{G_i'\}\langle G_j'\rangle d\eta$	➧	$U[\int_0^{\ell_e} \begin{Bmatrix} g_1' \\ g_2' \end{Bmatrix} \langle g_1' \; g_2'\rangle d\xi]$

Noting that,

$$g_1' = -\frac{1}{\ell_e}$$

$$g_2' = \frac{1}{\ell_e}$$

the elemental matrix becomes

$$\int_0^{\ell_e} \begin{bmatrix} (\frac{1}{\ell_e})^2 & -(\frac{1}{\ell_e})^2 \\ -(\frac{1}{\ell_e})^2 & (\frac{1}{\ell_e})^2 \end{bmatrix} d\xi \quad \Rightarrow \quad \frac{1}{\ell_e} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$

For operator E.2,

<u>global</u>	<u>local</u>
$\int_0^1 \{G_i\}\langle G_j' \rangle d\eta$	$\Rightarrow \quad U[\int_0^{\ell_e} \begin{Bmatrix} g_1 \\ g_2 \end{Bmatrix} \langle g_1' \; g_2' \rangle d\xi]$

Substituting in the local shape functions gives,

$$\int_0^{\ell_e} \begin{Bmatrix} (1 - \frac{\xi}{\ell_e}) \\ (\frac{\xi}{\ell_e}) \end{Bmatrix} \langle (-\frac{1}{\ell_e}) (\frac{1}{\ell_e}) \rangle d\xi$$

Carrying out the operations gives

$$\int_0^{\ell_e} \begin{bmatrix} (-\frac{1}{\ell_e} + \frac{\xi}{\ell_e}) & (\frac{1}{\ell_e} - \frac{\xi}{\ell_e}) \\ -(\frac{\xi^2}{2\ell_e^2}) & (\frac{\xi^2}{2\ell_e^2}) \end{bmatrix} d\xi \quad \Rightarrow \quad \frac{1}{2} \begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix}$$

For operator E.3,

<u>global</u>	<u>local</u>

$$\int_0^1 \{G_1\} \langle G_j \rangle d\eta \quad \Rightarrow \quad U\left[\int_0^{\ell_e} \begin{Bmatrix} g_1 \\ g_2 \end{Bmatrix} \langle g_1 \; g_2 \rangle d\xi \right]$$

Substituting in for the local shape functions

$$\int_0^{\ell_e} \begin{Bmatrix} (1 - \frac{\xi}{\ell_e}) \\ (\frac{\xi}{\ell_e}) \end{Bmatrix} \langle (1 - \frac{\xi}{\ell_e}) (\frac{\xi}{\ell_e}) \rangle d\xi$$

the elemental matrix becomes

$$\int_0^{\ell_e} \begin{bmatrix} (1 - 2\frac{\xi}{\ell_e} + \frac{\xi^2}{\ell_e^2}) & (\frac{\xi}{\ell_e} - \frac{\xi^2}{\ell_e^2}) \\ (\frac{\xi}{\ell_e} - \frac{\xi^2}{\ell_e^2}) & (1 - 2\frac{\xi}{\ell_e} + \frac{\xi^2}{\ell_e^2}) \end{bmatrix} d\xi \quad \Rightarrow \quad \frac{\ell_e}{3} \begin{bmatrix} 1 & \frac{1}{2} \\ \frac{1}{2} & 1 \end{bmatrix}$$

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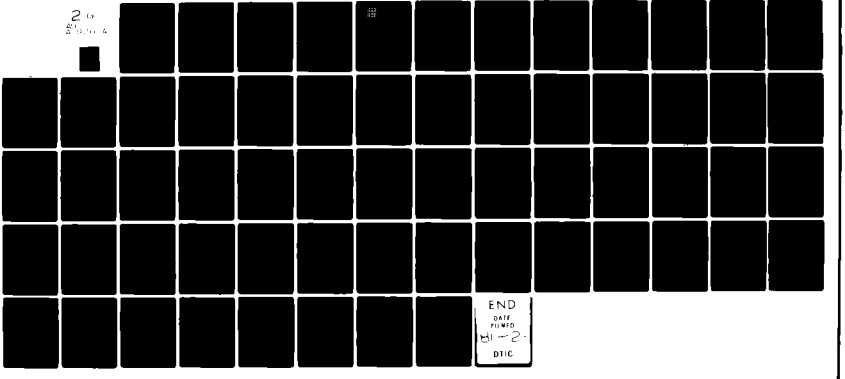

For operator E.4,

global		local

$$\int_0^1 \{G_i\}\langle G_j'\rangle \{\psi\}\langle G_j\rangle d\eta \quad \Rightarrow \quad U\{ \int_0^{\ell_e} \begin{matrix} g_1 \\ g_2 \end{matrix} \langle g_1' g_2'\rangle \begin{Bmatrix} \psi \\ \psi \end{Bmatrix} \langle g_1 g_2\rangle d\xi \}$$

Multiplying out the matrices, the expression becomes,

$$\int_0^{\ell_e} \begin{bmatrix} (g_1 g_1 g_1' \psi_{i-1} + g_1 g_1 g_2' \psi_i) & (g_1 g_1' g_2 \psi_{i-1} + g_1 g_2 g_2' \psi_i) \\ (g_1 g_1' g_2 \psi_{i-1} + g_1 g_2 g_2 \psi_i) & (g_1' g_2 g_2 \psi_{i-1} + g_2 g_2 g_2' \psi_i) \end{bmatrix} d\xi$$

Integrating each term separately,

$$\int_0^{\ell_e} g_1 g_1 g_1' d\xi = \int_0^{\ell_e} -\frac{1}{\ell_e} + \frac{2\xi}{\ell_e^2} - \frac{\xi^2}{\ell_e^3} d\xi = -\frac{1}{3}$$

$$\int_0^{\ell_e} g_1 g_1 g_2' d\xi = \int_0^{\ell_e} \frac{1}{\ell_e} - \frac{2\xi}{\ell_e^2} + \frac{\xi^2}{\ell_e^3} d\xi = \frac{1}{3}$$

$$\int_0^{\ell_e} g_1 g_1' g_2 d\xi = \int_0^{\ell_e} -\frac{\xi}{\ell_e^2} + \frac{\xi^2}{\ell_e^3} d\xi = -\frac{1}{6}$$

$$\int_0^{\ell_e} g_1 g_2 g_2' d\xi = \int_0^{\ell_e} \frac{\xi}{\ell_e^2} - \frac{\xi^2}{\ell_e^3} d\xi = \frac{1}{6}$$

$$\int_0^{\ell_e} g_1 g_1' g_2 d\xi = -\frac{1}{6}$$

$$\int_0^{\ell_e} g_1 g_2 g_2' d\xi = \frac{1}{6}$$

$$\int_0^{\ell_e} g_1' g_2 g_2 d\xi = \int_0^{\ell_e} -\frac{\xi^2}{\ell_e^3} d\xi = -\frac{1}{3}$$

$$\int_0^{\ell_e} g_1 g_2 g_2' d\xi = \int_0^{\ell_e} \frac{\xi}{\ell_e^3} d\xi = \frac{1}{3}$$

Substituting the values into the expression

$$\begin{bmatrix} (-\frac{1}{3}\Psi_{i-1} + \frac{1}{3}\Psi_i) & (-\frac{1}{6}\Psi_{i-1} + \frac{1}{6}\Psi_i) \\ (-\frac{1}{6}\Psi_{i-1} + \frac{1}{6}\Psi_i) & (-\frac{1}{3}\Psi_{i-1} + \frac{1}{3}\Psi_i) \end{bmatrix}$$

factoring out a - 1/3, the local matrix for the global operator becomes

$$\int_0^1 \{G_i\}\langle G_j\rangle\{\Psi\}\langle G_j\rangle d\eta \quad \Rightarrow \quad -\frac{1}{3}\begin{bmatrix} (\Psi_{i-1}-\Psi_i) & (\frac{\Psi_{i-1}-\Psi_i}{2}) \\ (\frac{\Psi_{i-1}-\Psi_i}{2}) & (\Psi_{i-1}-\Psi_i) \end{bmatrix}$$

For operator E.5,

<u>global</u>	<u>local</u>

$$\int_0^1 \{G_i\}d\eta \quad \Rightarrow \quad U\left[\int_0^{\ell_e} \begin{Bmatrix} g_1 \\ g_2 \end{Bmatrix} d\xi\right]$$

Substituting in the local shape function, and integrating, the expression becomes

$$\int_0^{\ell_e} \begin{Bmatrix} (1-\frac{\xi}{\ell_e}) \\ \frac{\xi}{\ell_e} \end{Bmatrix} d\xi \quad \Rightarrow \quad \frac{\ell_e}{2}\begin{Bmatrix} 1 \\ 1 \end{Bmatrix}$$

This last operator is used for the excitation vector as described in the FEM formulation.

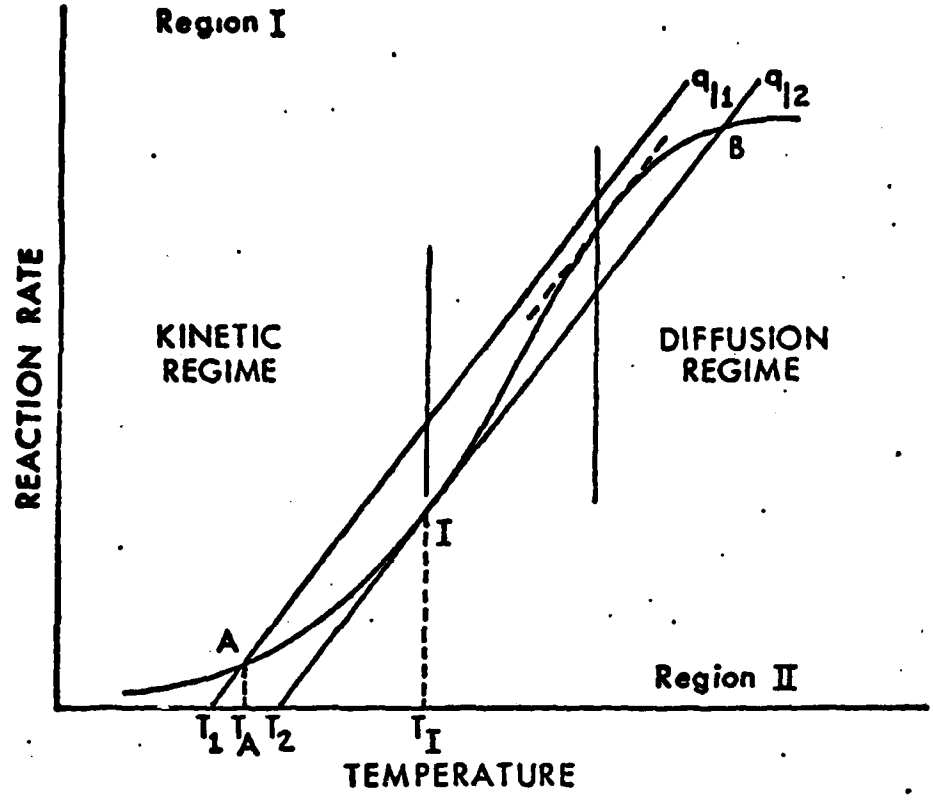

FIGURE 1 Semenov model of combustion.

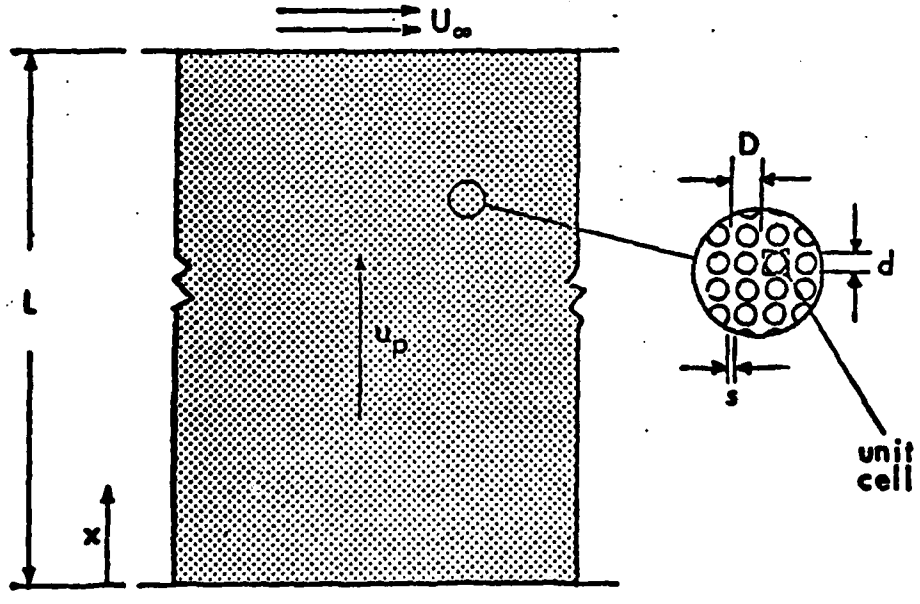

FIGURE 2 Idealized geometry of a fibrous graphite plate.

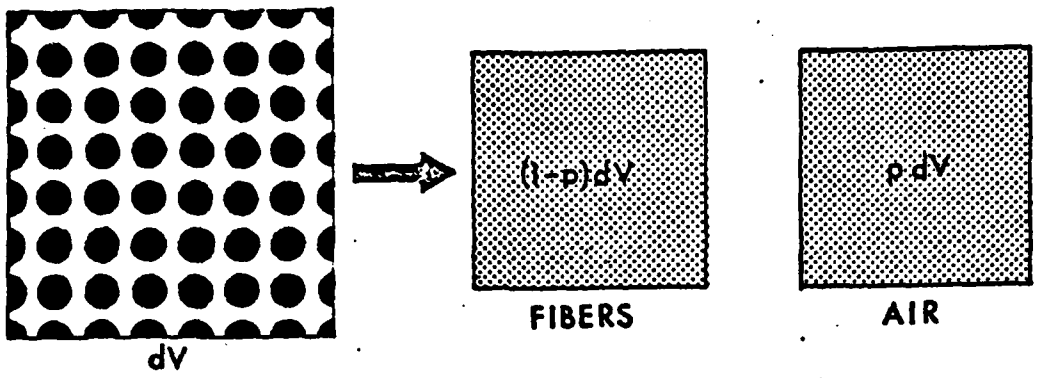

FIGURE 3 Separating a differential volume of porous medium into respective volumes of fiber and air.

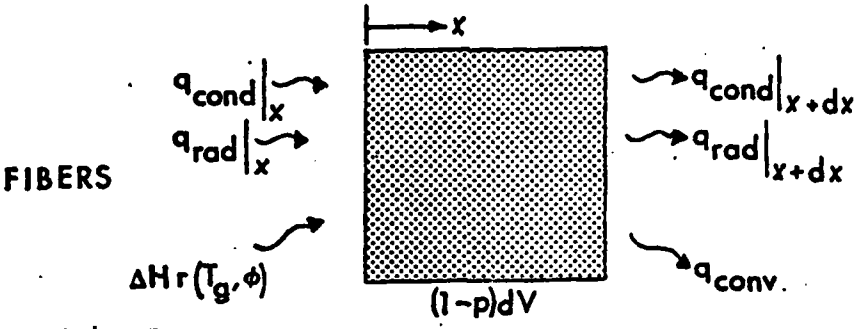

FIGURE 4 Energy balance on the fibers.

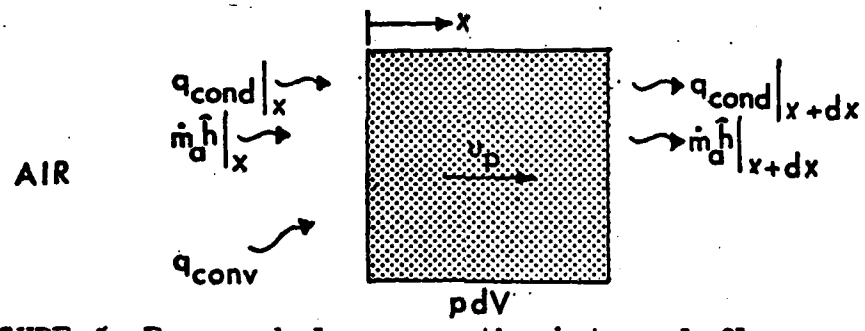

FIGURE 5 Energy balance on the internal flow.

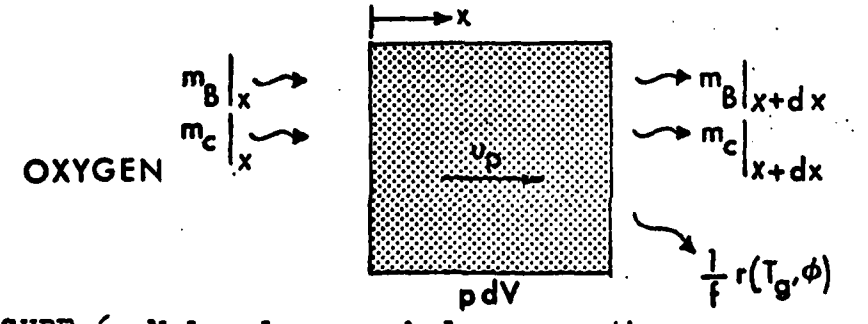

FIGURE 6 Molecule-mass balance on the oxygen.

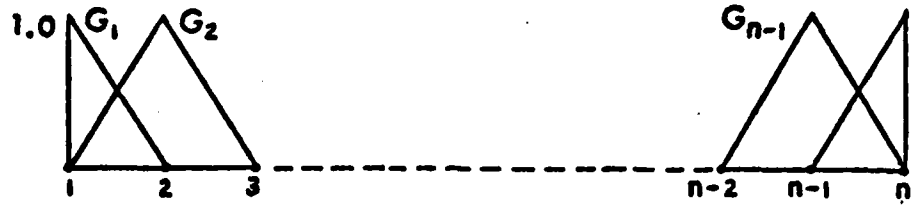

FIGURE 7 Linear shape functions for the Galerkin formulation of FEM.

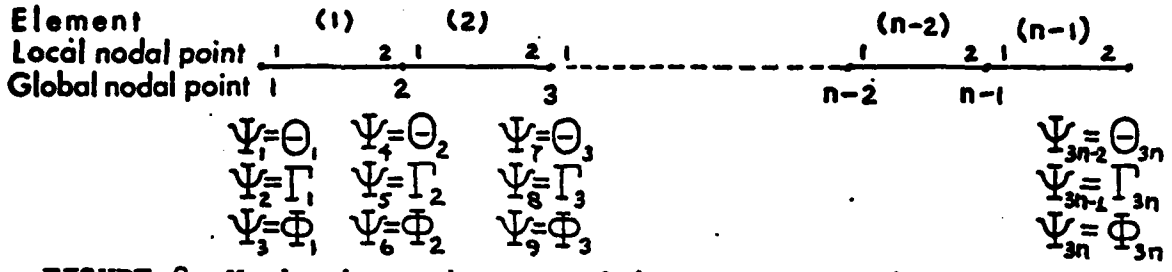

FIGURE 8 Numbering scheme used in system matrices.

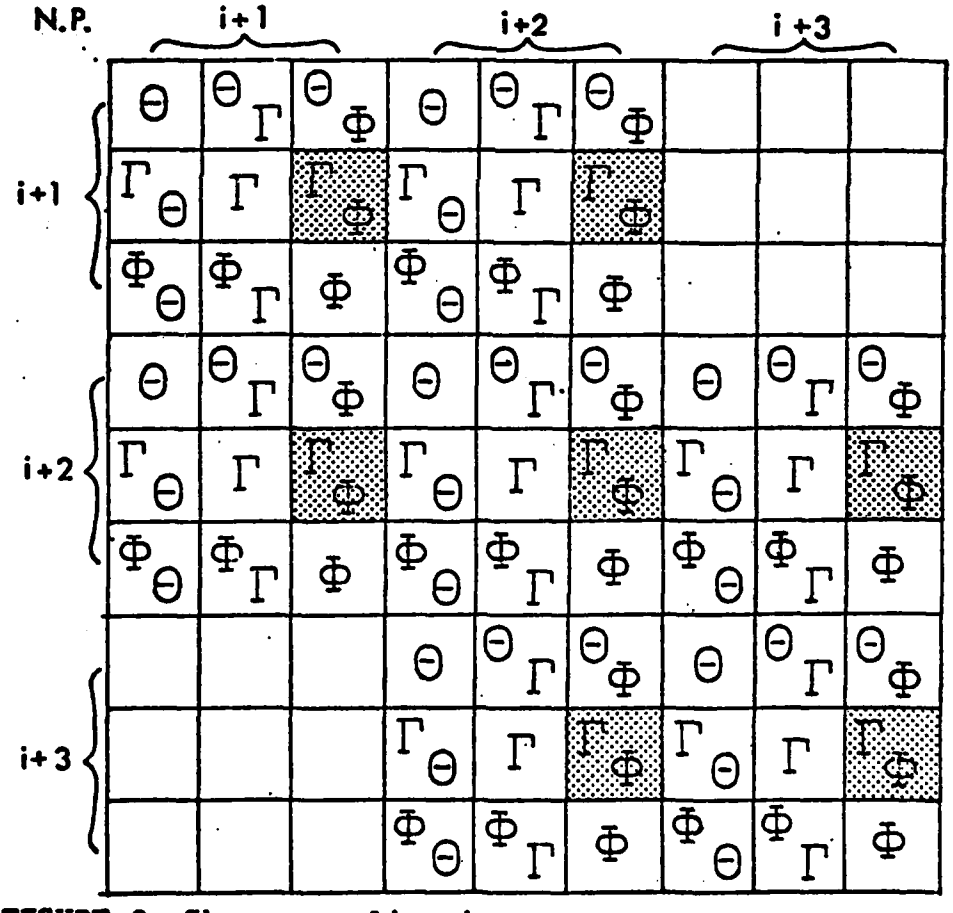

FIGURE 9 Shows coupling in system of p. d. e.

TABLE 1

SUMMARY OF RESULTS*

Case	U_∞ kt.	d in.	L in.	u_p ft./s.	ΔP psi.	Re_i	m $ft^2 \times 10^3$	p	h_{i_2} btu/ft²-hr-F	z ft^2/ft^3	Remarks
1	50.	.004	.25	.3745	.0597	.4487	.1652	.497	19.19	3016.	ignition @ 8.3s
2	90.	.004	.25	1.208	.1925	1.447	.1652	.497	34.06	3016.	extinction
3	120.	.004	.25	2.140	.3405	2.56	.1652	.497	45.04	3016.	extinction
4	20.	.004	.25	.060	.0096	.0719	.1652	.497	7.82	3016.	extinction
5	70.	.004	.25	.7235	.1168	.8778	.1652	.497	26.70	3016.	ignition @ 6.7s
6	10.	.004	.25	.015	.0024	.0180	.1652	.497	3.97	3016.	extinction
7	90.	.004	.5	.6039	.1925	.7236	.1652	.497	24.25	3016.	ignition @ 4.9s
8	90.	.004	1.0	.3019	.1925	.3618	.1652	.497	17.27	3016.	ignition @ 6.0s
9	50.	.002	.25	.6657	.0597	2.80	.5163	.8743	23.85	1508.	extinction
10	50.	.0048	.25	.2813	.0597	.156	.0689	.276	13.62	3619.	extinction
11	90.	.004	1.5	.2013	.1925	.2412	.1652	.497	14,16	3016.	ignition @ 6.6s
12	90.	.004	2.0	.151	.1925	.1809	.1652	.497	12.29	3016.	ignition @ 8.0s
13	90.	.004	4.0	.0755	.1925	.0905	.1652	.497	8.75	3016.	ignition
14	90.	.004	6.0	.0503	.1925	.0603	.1652	.497	7.18	3016.	ignition

* For D=.005" and initial conditions of Figure 10

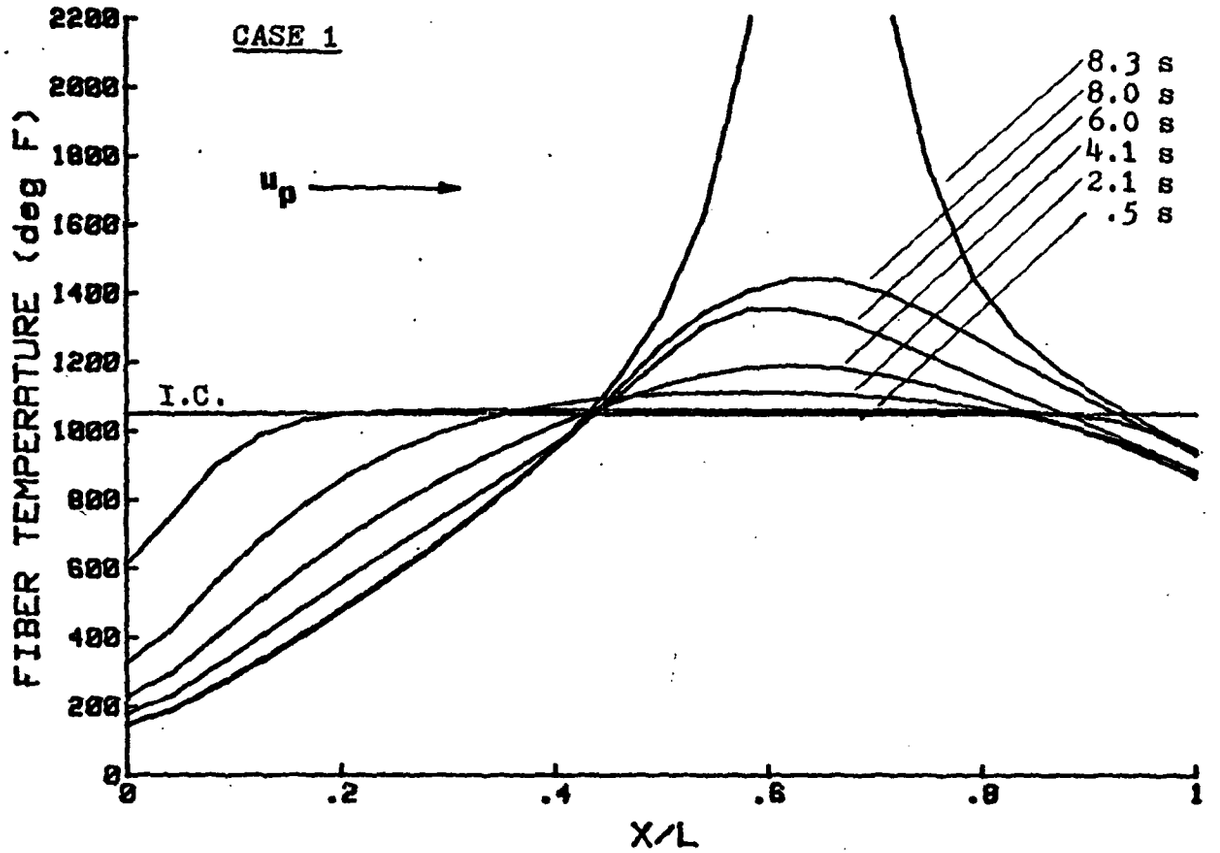

FIGURE 10 Fiber temperature response of Case 1 (U_∞=50kt.; d=.004"; L=.25").

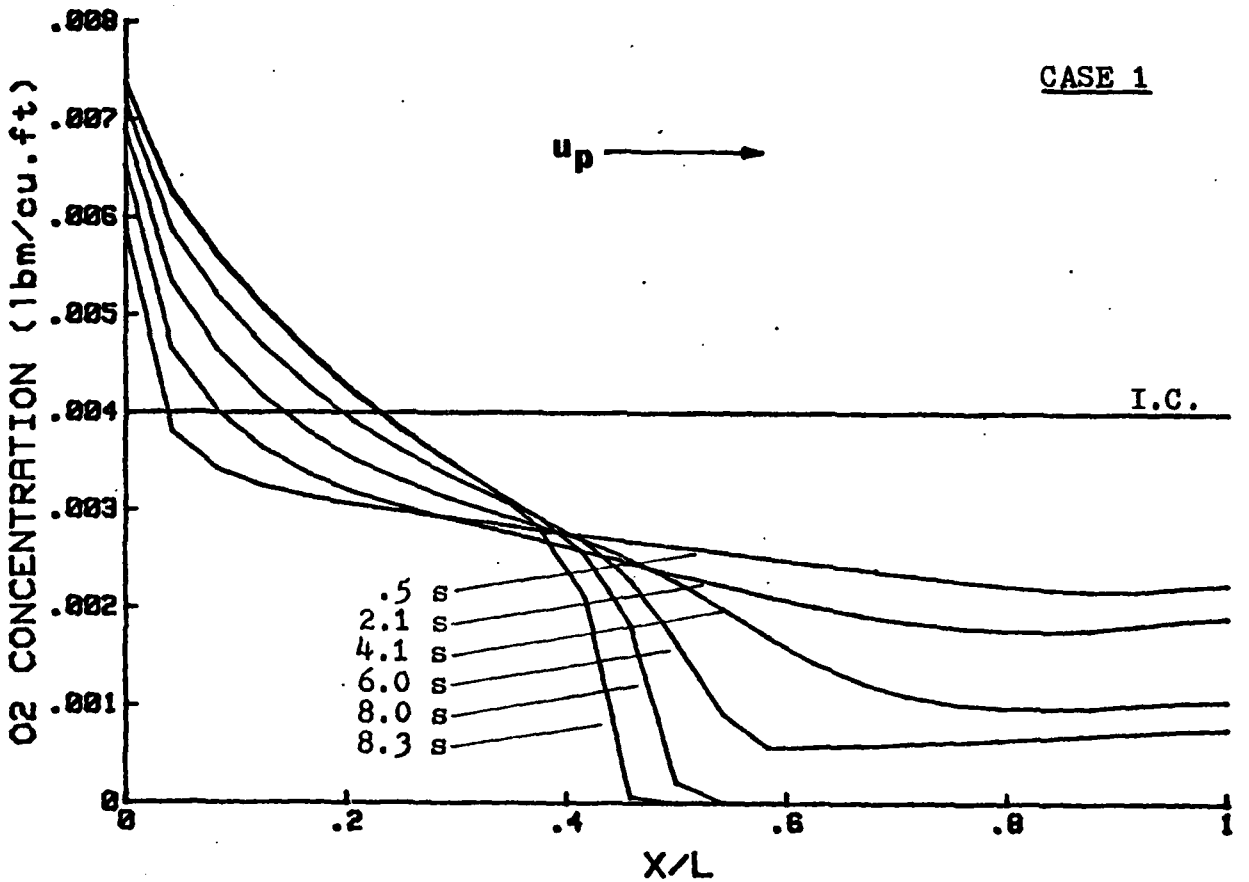

FIGURE 11 Oxygen concentration response of Case 1 (U_∞=50kt.; d=.004"; L=.25").

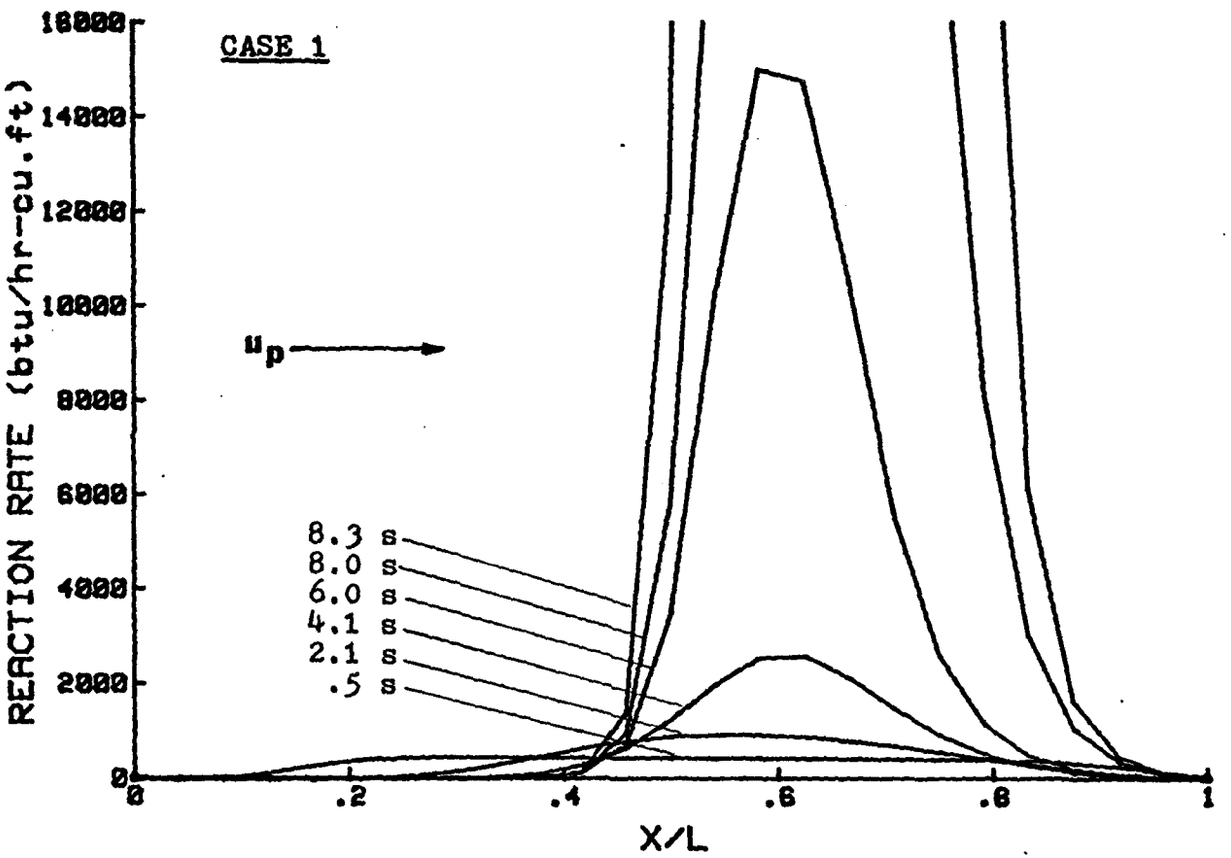

FIGURE 12 Observed reaction rate for Case 1.

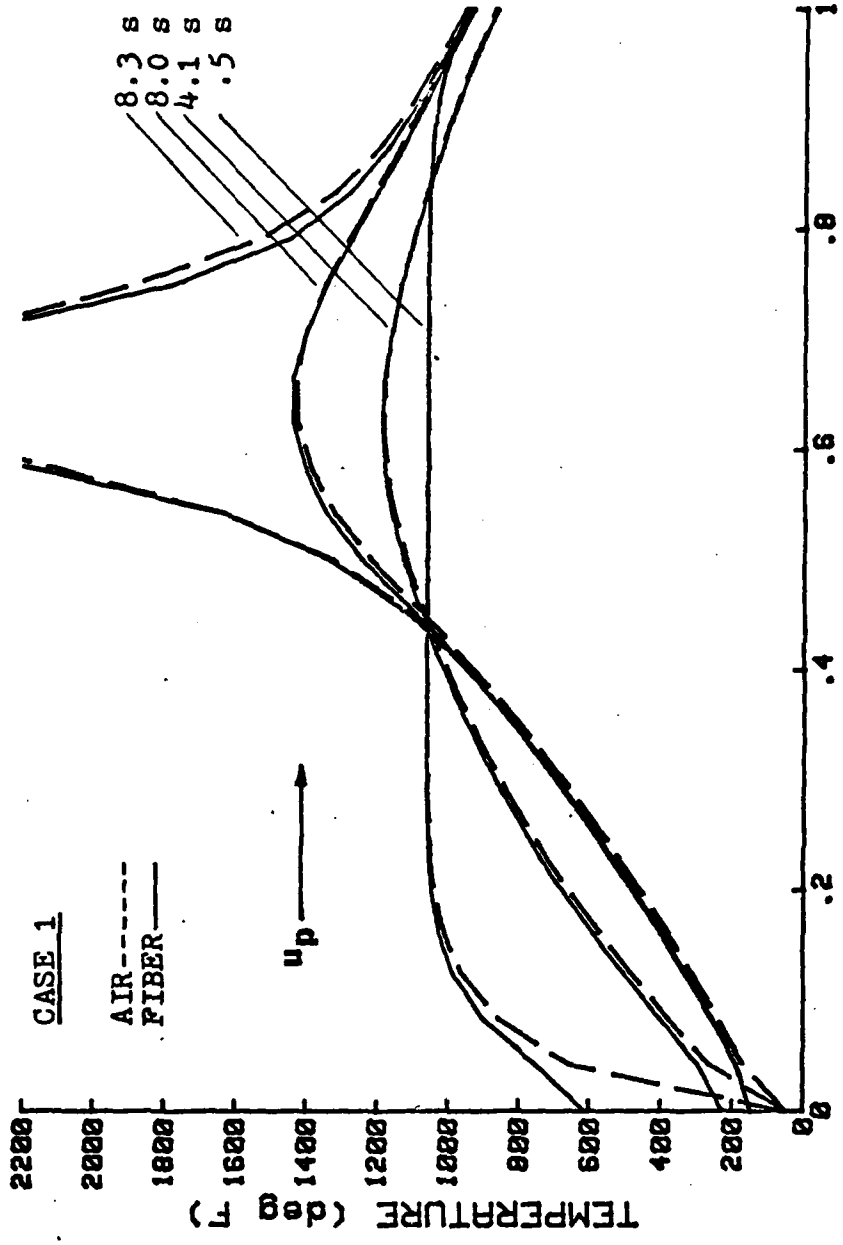

FIGURE 13 Flow temperature follows the fiber temperature.

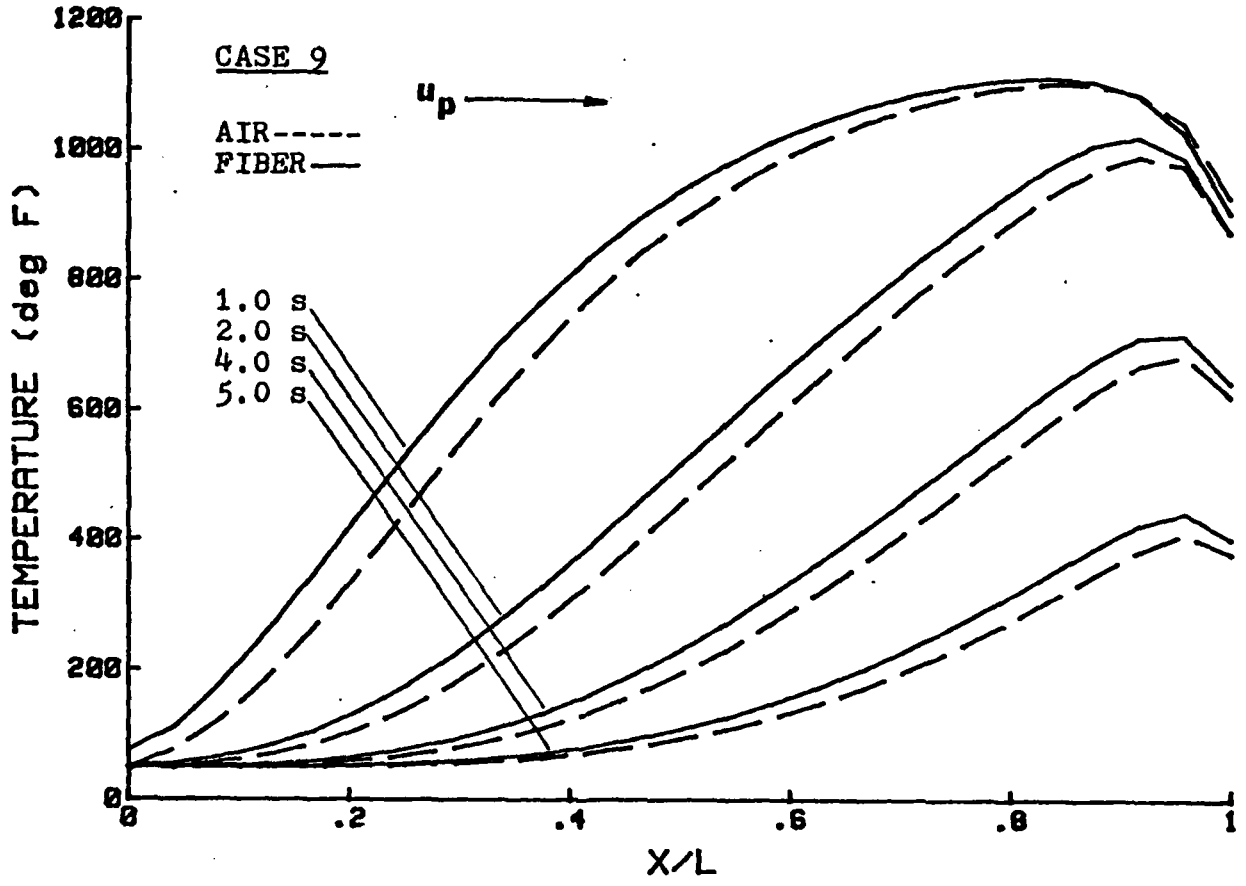

FIGURE 14 Flow and fiber temperature difference at high porosity and flow rate (for Case 9, p=.87, U_∞=90kt.).

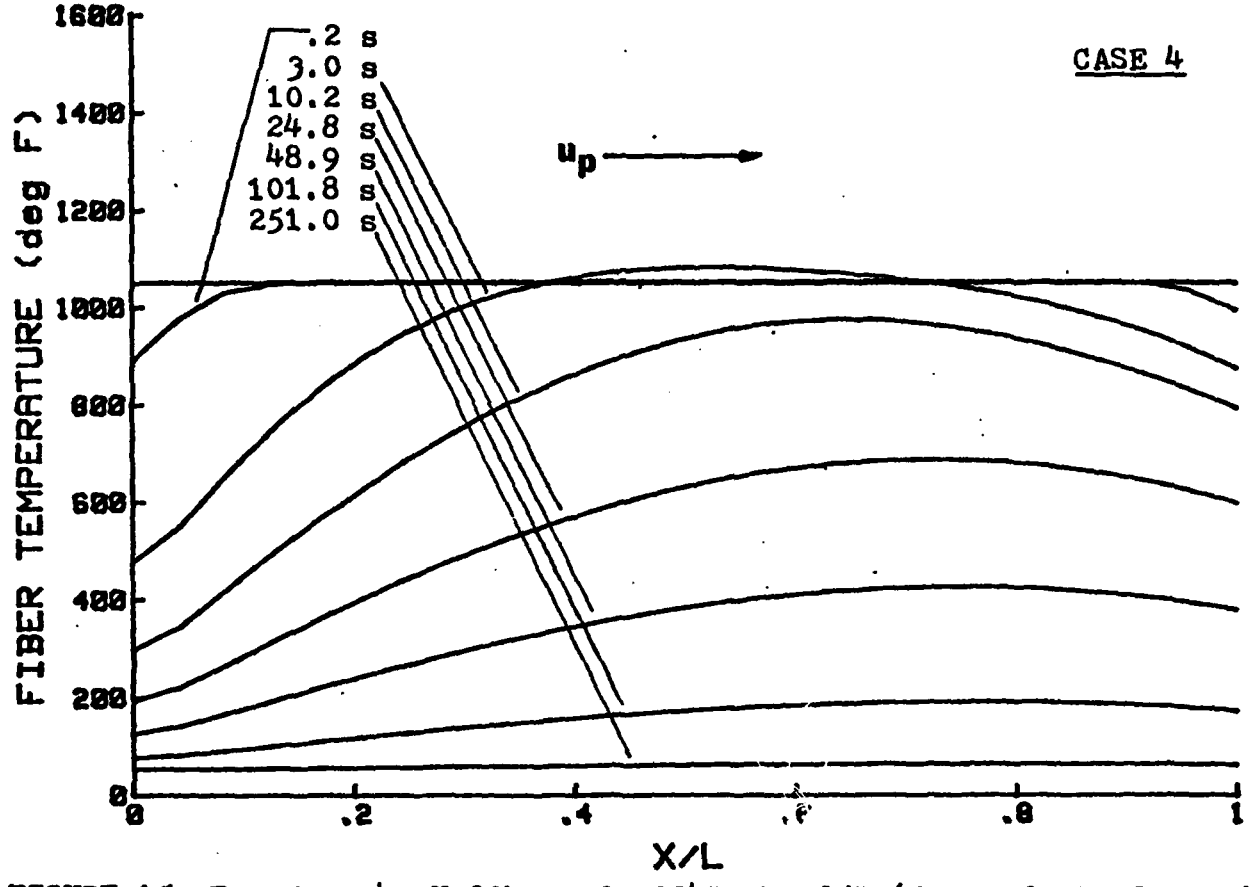

FIGURE 15 For Case 4, U_∞=20kt., d=.004", L=.25" (for effect of varying exterior velocity, U_∞, compare Figures 15, 16 and 17).

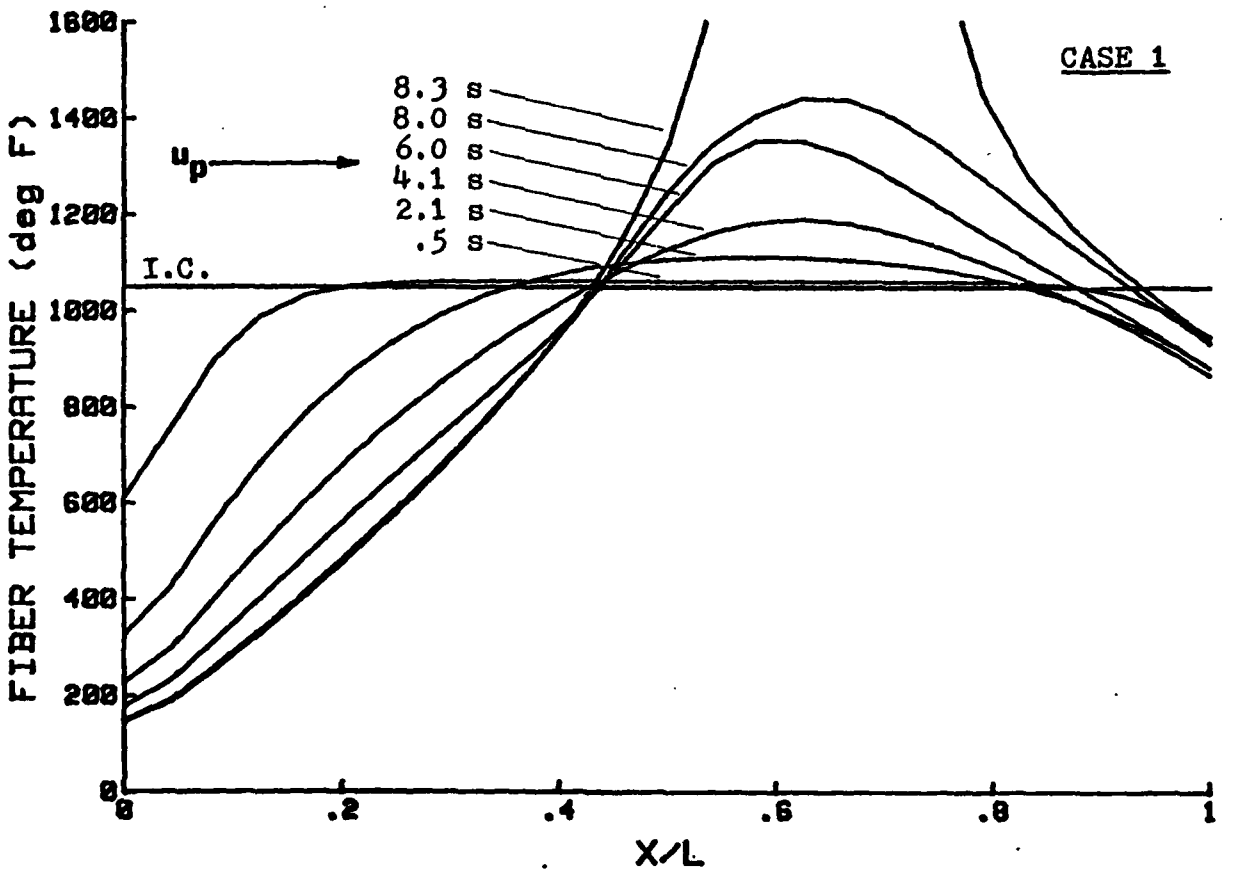

FIGURE 16 For Case 1, U_g=50kt., d=.004", L=.25".

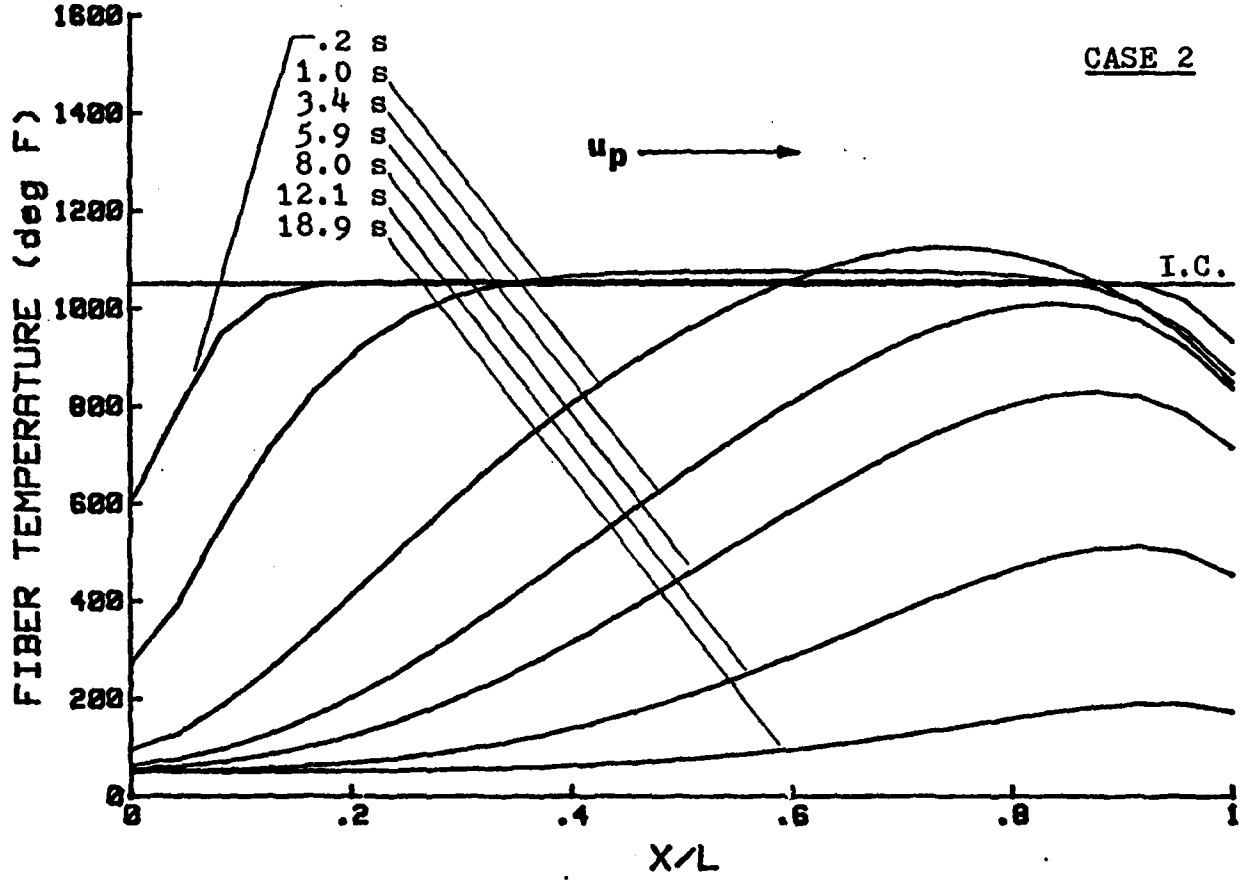

FIGURE 17 For Case 2, U_∞=90kt., d=.004", L=.25".

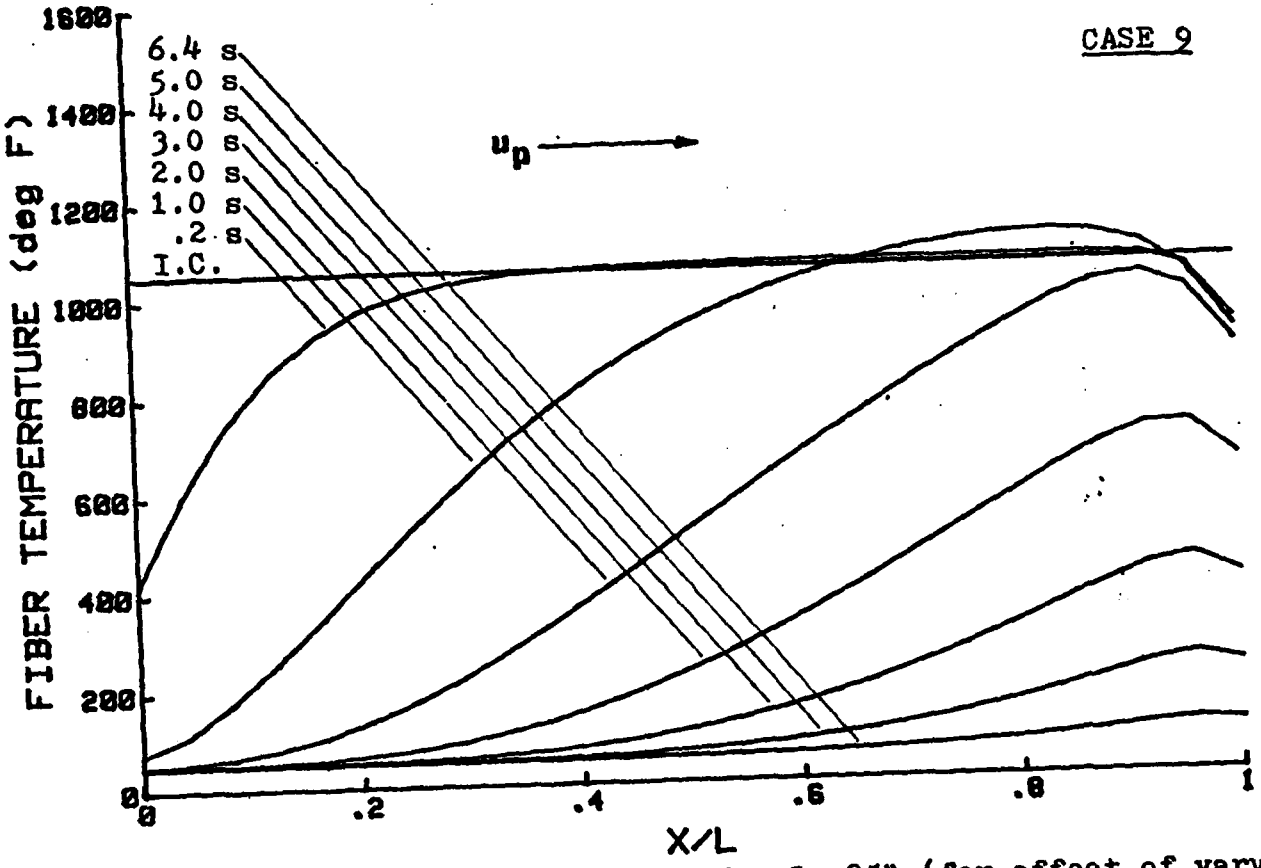

FIGURE 18 For Case 9, U_{∞}=50kt., d=.002", L=.25" (for effect of varying fiber diameter, d, compare Figures 16, 18 and 19).

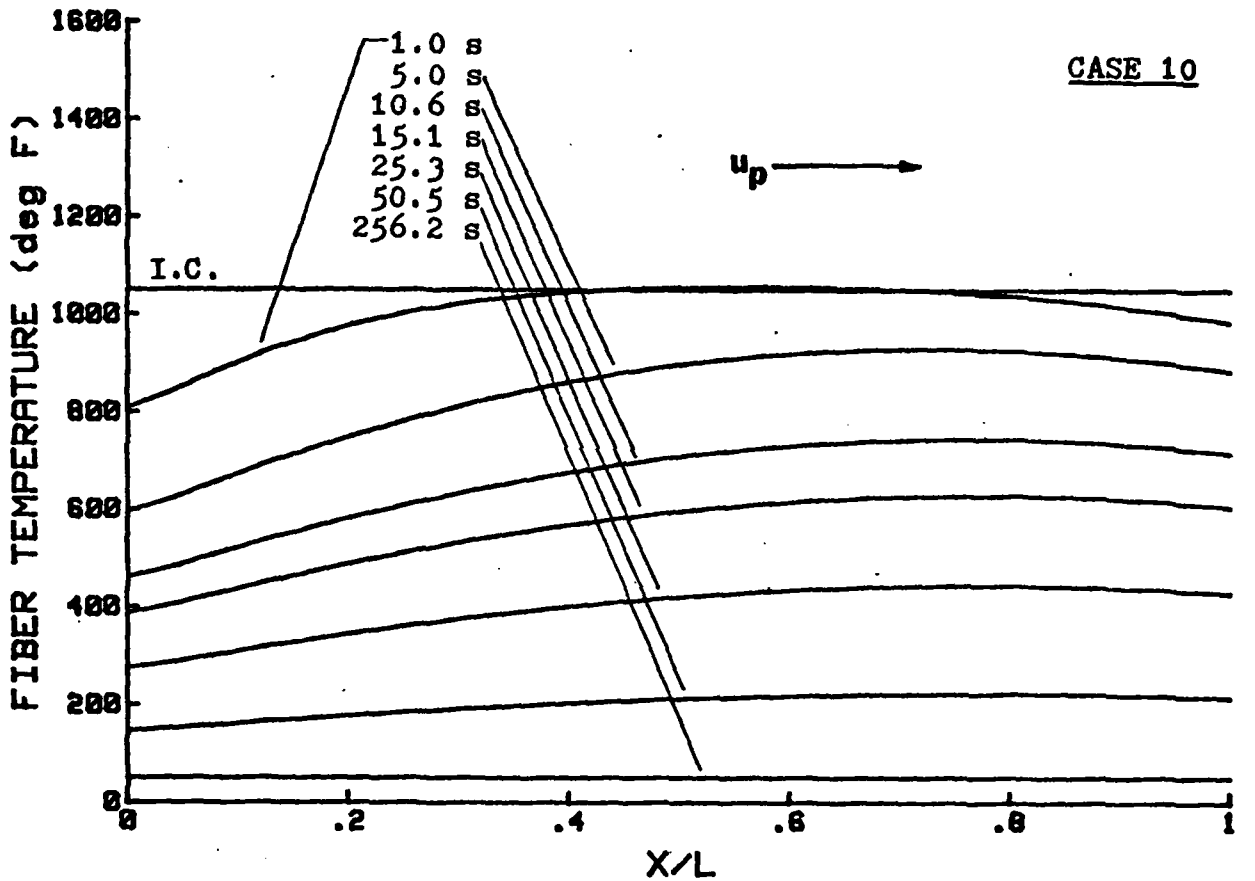

FIGURE 19 For Case 10, U_∞=50kt., d=.0048", L=.25".

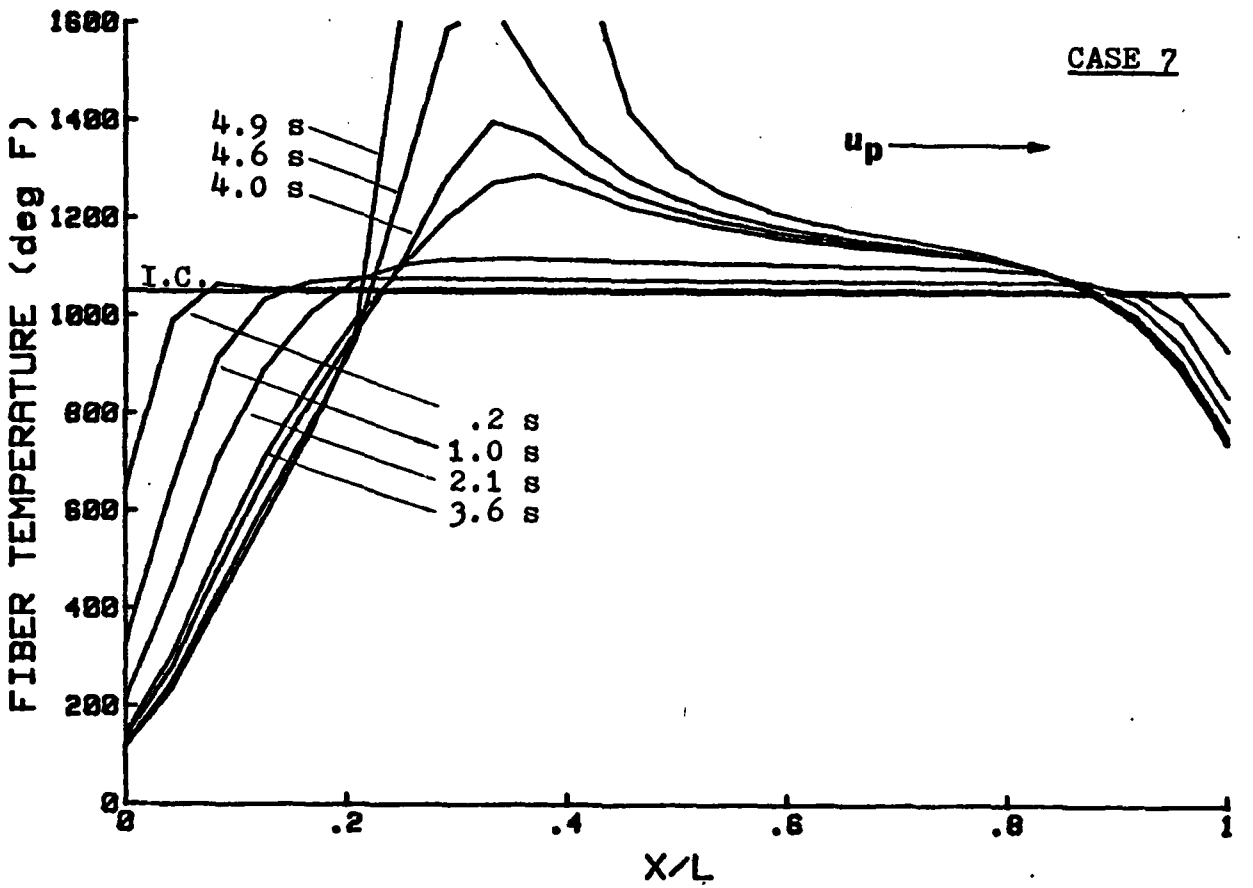

FIGURE 20 For Case 7, U_x=90kt., d=.004", L=.5" (for effect of varying plate thickness, L, compare Figures 17, 20 and 21).

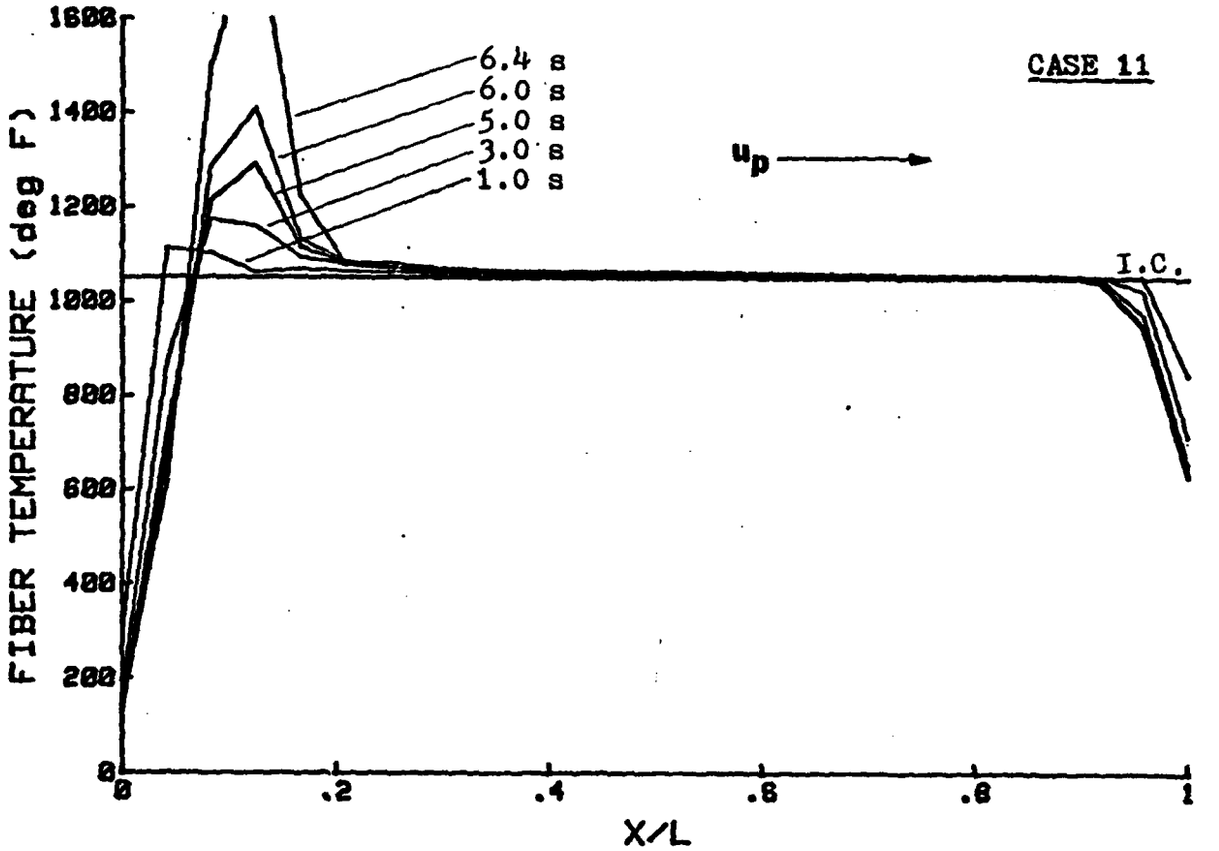

FIGURE 21 For Case 11, U_∞=90kt., d=.004", L=1.5".

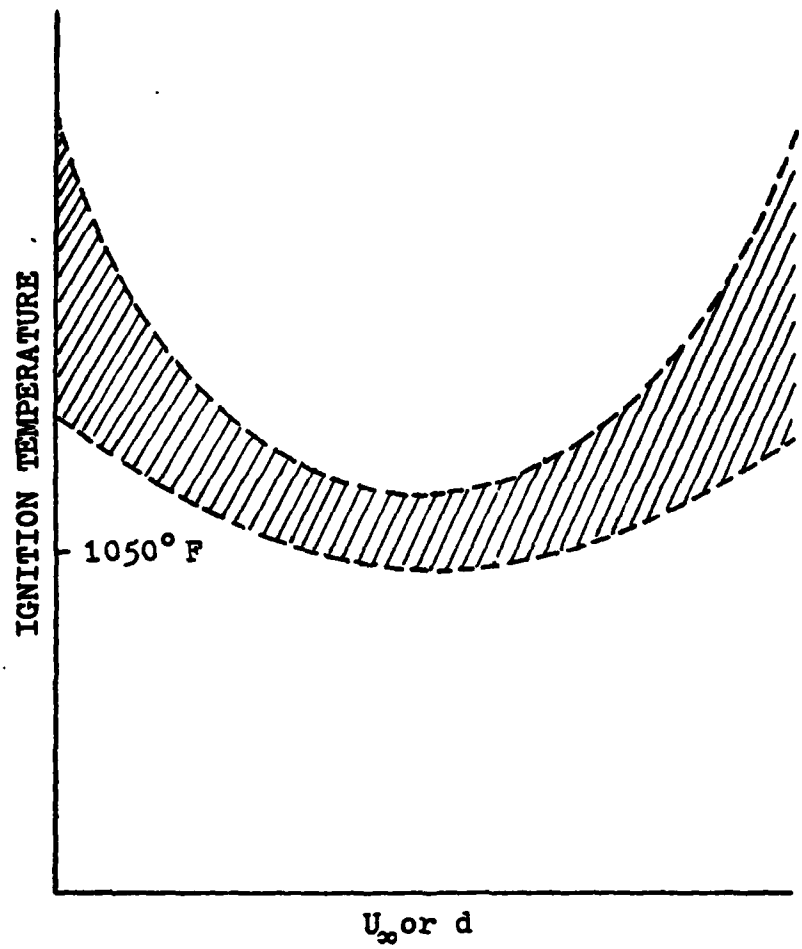

FIGURE 22 Shaded region represents shape of ignition temperature curve as a function of U_∞ or d.

```
C     ***************************************************************
C     *   ONE-DIM'L TRANSIENT HEAT TRANSFER IN POROUS GRAPHITE      *
C     *                    WITH COMBUSTION                          *
C     ***************************************************************
C
C
C PARAMETER DEFINITIONS:
C
C    NNP=NUMBER OF NODAL POINTS          UINF1=EXTERIOR SURF VEL. (KT)
C    TAMB=AMBIENT TEMP. (F)              PAMB1=AMBIENT PRESSURE (PSI)
C    TORT=TORTUOSITY                     D1=FILAMENT DIA. (IN.)
C    SPACE1=FLY THICKNESS (IN.)          HLENTH=REFERENCE LENGTH FOR
C                                          CONVECTION HEAT TRANSFER
C                                          COEFF. (FT.)
C    XLENT1=PLATE THICKNESS (IN.)        RGAS=GAS CONSTANT FOR AIR (LBF*
C                                          FT.PER LBM*DEG-R)
C    GCOND=CONDUCTIVITY OF BULK          EMIS=EMISSIVITY OF FIBER
C      GRAPHITE (BTU PER FT.*HR*F)
C    SPHTG=SPEC.HEAT OF GRAPHITE         SPHTA=SPEC.HEAT OF AIR (BTU PER
C      (BTU PER LBM*F)                     LBM*F)
C    HSURFL=AFFECX. CONV. HEAT           CAMB1=AMBIENT CONC. OF OXYGEN
C      TRANS. COEFF. AT X=0 (BTU         ROG=MASS DENSITY OF BULK GRAPHITE
C      PER HR*FT**2*F)                     (LBM PER FT**3)
C    T=TIME STEP AT WHICH PRINT          HMAX=MAX. INTEGRATION STEP
C      OUT OF VARIABLES DESIRED            ALLOWABLE (SEC.)
C      (SEC.)
C    TSTART=START TIME FOR PROBLEM (SEC); USED FOR BOOKEEPING
C      SUCH AS A RESTART FROM PREVIOUS PROBLEM (INPUT 0.0
C      IF INITIAL RUN).
C    X(I)=NON-DIMEN. NODAL POINT LOCATIONS (VALUES BETWEEN 0.0-
C      1.0)
C    CHI(1,I)=ARRAY HOLDING INITIAL CONDITIONS (DEG-F;LBM PER FT**3);
C      TEMP-G ENTERED INTO LOC. (1,1),(1,4)...,(1,3*NNP-2);  TEMP-A
C      ENTERED INTO (1,2),(1,5)...,(1,3*NNP-1); CONC-A ENTERED INTO
C      (1,3),(1,6)...,(1,3*NNP); DATA FILE STACKED WITH TEMP-G VALUES
C      FIRST, THEN TEMP-A, FINALLY CONC-A.
C    IELEM=CODE FOR N.P. DISTRIBUTION (0=ENTER NODAL POINT, X/L:
C      1=AUTOMATICALLY DIVIDES XLENT1 INTO NNP NODAL POINTS)
C
C FOR INPUT OF DATA LOOK AT SAMPLE INPUT FILE IN THESIS.
C
C
C PROGRAM CALCULATES FOLLOWING PROPERTIES FOR AMBIENT CONDITIONS
C AT START OF PROGRAM:
C
C  DELP1=PRESSURE DIFF. ACROSS PLATE (PSI)
C  2=SURF.AREA OF FIBER PER UNIT VOLUME (FT**2 PER FT**3)
```

```
C   PCRCS=PCRCSITY CF PLATE                                                    0047
C   FERM=FERMIABILITY OF PLATE (SQ.FT.)                                        0048
C   ZPORE=NUMBER CF PORES PER UNIT SURFACE AREA (PER SQ.FT.)                   0049
C   U=AVG.PORE VELOCITY (FT.PER SEC)                                           0050
C   DEL1=AVG.PORE DIAMETER (IN.)                                               0051
C   RCA=DENSITY CF AIR (LBM PER FT**3)                                         0052
C   ACOND=CONDUCTIVITY OF AIR (BTU PER FT*HR*DEG-F)                            0053
C   VISC=VISCOSITY CF AIR (LBM PER FT**2*HR)                                   0054
C   CCND=CONDUCTIVITY OF PLATE (BTU PER FT*HR*DEG-F)                           0055
C   RADCON=RADIATION COEFF. TO MULTIPLY T-CUBED FOR EQUIVALENT                 0056
C     CONDUCTIVITY (BTU PER FT*HR*DEG-R**4)                                    0057
C   RCG1=DENSITY CF POROUS MEDIUM (LBM PER FT**3)                              0058
C   RE=REYNOLDS NUMBER FOR EXTERIOR FLOW                                       0059
C   REIN=INTERNAL REYNOLDS NUMBER                                              0060
C   CONV=INTERNAL CONVECTION HEAT TRANSFER COEF.(BTU PER HR*FT**2*F)           0061
C   HSURFR=HEAT TRANSFER COEF. AT RIGHT SURFACE (BTU PER HR*FT**2*F)           0062
C                                                                              0063
C                                                                              0064
C  FOLLOWING PROPERTIES ARE EVALUATED AT THE PREVIOUS TIME STEP IN             0065
C  S.R. FORM2 FOR EACH NODAL POINT:                                            0066
C                                                                              0067
C   1. VISCOSITY CF AIR (VISC2)                                                0068
C   2. CONDUCTIVITY CF AIR (ACOND2(I))                                         0069
C   3. DENSITY CF AIR (ROA2(I))                                                0070
C   4. AVG.PORE VELOCITY (U2(I))                                               0071
C   5. INTERNAL REYNOLDS NUMBER (REIN)                                         0072
C   6. INTERNAL CONVECTION HEAT TRANS.COEF. (CONV2(I))                         0073
C   7. EQUIVALENT CONDUCTIVITY DUE TO RADIATION (CCND2(I))                     0074
C   8. CONDUCTIVITY OF PLATE (CCND2(I), BOTH RAD. AND THERM.COND.              0075
C        INCLUDED IN TERM)                                                     0076
C   9. DIFFUSIVITY COEFFICIENT (TVGA(I))                                       0077
C  10. HEAT GENERATION TERM (RATEH)                                            0078
C  11. OXYGEN CONSUMPTION TERM (RATE)                                          0079
C                                                                              0080
C                                                                              0081
C  MAIN PROGRAM **********************************                             0082
C                                                                              0083
C                                                                              0084
C                                                                              0085
C  INPUT DATA****                                                              0086
C                                                                              0087
      REAL*8 ZK,ZDCT,GAMMA,GAM                                                 0088
      EXTERNAL DIFFUN,JACMAT,DCASUB,COPYZ,NUITSL,DERVAL                        0089
      COMMON ZK(75,75),ZDCT(75,75),XLENTH,CCND,RADCON,CONV,Z,ROG,              0090
     XDELP,PCRCS,CHI(7,75),TAMB,CAMB,F(75),                                    0091
     XPAMB,ACACC(25,4),BDCT(25,4),BSH(25,4),X(75),U,CD(25,4),                  0092
     XRGAS,BCECC(25,4),CC(25,4),ADCT(25,4),BETA,GCCND,D,SPHTG,ROA,SPHTA,       0093
     XRGAS,BCECC(25,4),CC(25,4),ADCT(25,4),BETA,GCCND,D,SPHTG,ROA,SPHTA,       0094
```

```
      XCOND2(25),TORT,CC2(25,4),SPHT,ZMASS(75),PERM,VISC,                    0095
      XU2(25),NNP,NNPA,NNPE,NNFC,NEL,ICOR(75,2),IJK                          0096
       DIMENSION C(75),W(7500),YL(1),X2(1),Y4(1),Y1(25),Y2(25),Y3(25),       0097
      XX1(25),FACTK(75),FCF(75)                                              0098
       READ(5,5)  IELEM                                                      0099
5      FORMAT(I1)                                                            0100
       WRITE(6,6)  IELEM                                                     0101
6      FORMAT('C',4I1)                                                       0102
CCCCC                                                                        0103
CCCCC                                                                        0104
CCCCC                                                                        0105
C  GEOMETRY OF DOMAIN (1-DIMEN)****                                          0106
C                                                                            0107
       READ(5,10) NNP                                                        0108
10     FORMAT(I2)                                                            0109
       NEL=NNP-1                                                             0110
       IF(IELEM.EQ.1) GO TO 20                                               0111
       READ(5,15)  (X(I),I=1,NNP)                                            0112
15     FORMAT(F12.7)                                                         0113
       GO TO 35                                                              0114
20     X(1)=0.0                                                              0115
       DO 30  I=2,NNP                                                        0116
       J=I-1                                                                 0117
       X(I)=X(J)+1.0/FLOAT(NEL)                                              0118
30     CONTINUE                                                              0119
35     WRITE(6,40)                                                           0120
40     FORMAT('0','NODAL PT.     X-POSITION')                                0121
       WRITE(6,45)  (I,X(I),I=1,NNP)                                         0122
45     FORMAT(' ',4X,I2,9X,F5.3/)                                            0123
CCCCC                                                                        0124
CCCCC                                                                        0125
CCCCC                                                                        0126
C  PHYSICAL PROPERTIES****                                                   0127
C                                                                            0128
       READ(5,50) T,HMAX,ISTART,UINF1,TAMB,PAMB1,TORT,D1,SPACE1,HLENTH,      0129
      XXLENTH,RGAS,GCOND,EPIS,RCG,SPHTG,SPHTA,HSURFL,CAMB1                   0130
50     FORMAT(G12.6)                                                         0131
       UINF=UINF1*1.688                                                      0132
       PAMB=PAMB1*144.0                                                      0133
       DEL1=(2.0*SPACE1-D1)/2.0                                              0134
       DEL=DEL1/12.0                                                         0135
       D=D1/12.0                                                             0136
       SPACE=SPACE1/12.0                                                     0137
       XLENTH=XLENTH/12.0                                                    0138
       TABS=TAMB+459.7                                                       0139
       BETA=D/SPACE                                                          0140
       PORCS1=3.1416/4.0*(BETA**2)                                           0141
       POROS=1.0-PORCS1                                                      0142
```

```
      ZPCRE=(1.C/SPACE1)**2                                                     0143
      DELP=PAMB*(1.C-EXP(-UINF**2/(64.4*RGAS*TABS)))                            0144
      ROA=PAMB/(RGAS*TABS)                                                      0145
      PERM=PCPCS*DEL**2/(96.0*TCRT**2)                                          0146
      VISC=-1.041E-8*TAMB**2+6.0288E-5*TAMB+.0394                               0147
      U=4.17E8*PERM*(DELP/XLENTH)/(VISC*POROS)                                  0148
      ACCNC=-3.232E-9*TAMB**2+2.412E-5*TAMB+.0131                               0149
      ZKAPPA=ACCNC/CCOND                                                        0150
      GAMMA=(1.C/BETA)*ZKAPPA/(1.0-ZKAPPA)                                      0151
      GAM=DSQRT(1.0-GAMMA*GAMMA)                                                0152
      FI1=DLOG((1.0+GAM)/GAMMA)                                                 0153
      GM=1.C-GAMMA*GAMMA                                                        0154
      PI2=1.C+GAMMA/SQRT(GM)*PI1                                                0155
      CCND=ACCNC/(1.0-BETA*PI2)                                                 0156
      Z=.5*3.1416*D/SPACE**2                                                    0157
      RADCCN=4.0*1.73E-9*DEL*EMIS/(2.0-EMIS)                                    0158
      UINFPR=UINF1*6.076E3                                                      0159
      RE=UINFPR*XLENTH*RCA/VISC                                                 0160
      IF(RE.GT.5.0E5) GO TO 47                                                  0161
      HSURFR=.5856*SQRT(RE)*ACCND/HLENTH                                        0162
      GO TO 48                                                                  0163
   47 HSURFR=(.032853*(RE**.8)-754.7)*ACOND/HLENTH                              0164
   48 G=L*PCPCS*RCA                                                             0165
      REIN=G/(2*VISC*.91)                                                       0166
      SPHT=PCPCS*SPHTA+(1-PCPCS)*SPHTG                                          0167
      CONV=.91**2*SPHT*G/(REIN**.51*(SPHTA*VISC/ACCND)**.66)                    0168
      DELF1=DELF/144.0                                                          0169
      L3=U/3600.0                                                               0170
      ROG1=RCG*(1.0-POROS)                                                      0171
      WRITE(6,49)                                                               0172
   49 FORMAT('0',/,6X,'THE FOLLOWING PROPERTIES ARE INPUT:'/)                   0173
      WRITE(6,51) T                                                             0174
   51 FORMAT(' ','APPROX. TIME INTERVAL FOR INTEGRATION OUTPUT=',               0175
     XE10.4,' SEC.')                                                            0176
      WRITE(6,52) HMAX                                                          0177
   52 FORMAT('0','MAX. ALLOWABLE STEP FOR INTEGRATION=',E10.4,' SEC.')          0178
      WRITE(6,53) TSTART                                                        0179
   53 FORMAT('0','START TIME FOR PROBLEM=',E10.4,' SEC.')                       0180
      WRITE(6,54) UINF1                                                         0181
   54 FORMAT('0','VELOCITY OVER EXTERIOR RIGHT SIDE=',E10.4,' KNOTS')           0182
      WRITE(6,56) TAMB                                                          0183
   56 FORMAT('0','AMBIENT TEMPERATURE=',E10.4,' DEG-F')                         0184
      WRITE(6,58) PAMB1                                                         0185
   58 FORMAT('0','AMBIENT PRESSURE=',E10.4,' PSI.')                             0186
      WRITE(6,66) TORT                                                          0187
   66 FORMAT('0','TORTUOUSITY (LENGTH OF PATH PER LENGTH THICKNESS OF ME        0188
     XDIUM)=',E10.4)                                                            0189
      WRITE(6,70) D1                                                            0190
```

```
 70    FORMAT('C','FILAMENT DIAMETER=',E10.4,' INCHES')                      0191
       WRITE(6,72) HLENTH                                                    0192
 72    FORMAT('0','SIDE LENGTH OF SQUARE POROUS PLATE=',E10.4,' FT.')        0193
       WRITE(6,71) SPACEI                                                    0194
 71    FORMAT('0','THICKNESS OF SINGLE MATIX-FILAMENT LAMINATE=',E10.4,'     0195
      1INCHES')                                                              0196
       WRITE(6,74) XLENTI                                                    0197
 74    FORMAT('C','THICKNESS OF POROUS PLATE=',E10.4,' INCHES')              0198
       WRITE(6,76) RGAS                                                      0199
 76    FORMAT('0','GAS CONSTANT OF AIR=',E10.4,' LBF*FT. PER LBM*DEG-R')     0200
       WRITE(6,77) CAMBI                                                     0201
 77    FORMAT('C','AMBIENT CONCENTRATION OF OXYGEN=',E10.4,' LBM PER CU.F    0202
      1XT.')                                                                 0203
       WRITE(6,78) GCOND                                                     0204
 78    FORMAT('C','CONDUCTIVITY OF FILAMENT MATERIAL=',E10.4,' BTU PER FT    0205
      1X*HR*DEG-F')                                                          0206
       WRITE(6,80) EMIS                                                      0207
 80    FORMAT('0','EMISSIVITY OF FILAMENT MATERIAL=',E10.4)                  0208
       WRITE(6,82) RCG                                                       0209
 82    FORMAT('C','MASS DENSITY OF FILAMENT MATERIAL=',E10.4,' LBM PER CU    0210
      1.FT.')                                                                0211
       WRITE(6,84) SPHTG                                                     0212
 84    FORMAT('C','SPECIFIC HEAT OF FILAMENT MATERIAL=',E10.4,' BTU PER L    0213
      1BM*DEG-F')                                                            0214
       WRITE(6,86) SPHTA                                                     0215
 86    FORMAT('0','SPECIFIC HEAT OF AIR=',E10.4,' BTU PER LBM*DEG-F')        0216
       WRITE(6,87) FSURFL                                                    0217
 87    FORMAT('C','CONVECTION HEAT TRANSFER COEF. ON STILL SIDE=',E10.4,'    0218
      1 BTU PER FT**2*HR*DEG-F')                                             0219
       WRITE(6,88)                                                           0220
 88    FORMAT('C',/,6X,'THE FOLLOWING PROPERTIES ARE CALCULATED FOR AMBIE    0221
      1NT CONDITIONS:')                                                      0222
       WRITE(6,90) DELP1                                                     0223
 90    FORMAT('0','PRESSURE DIFFERENTIAL ACROSS PLATE=',E10.4,' PSI.')       0224
       WRITE(6,91) Z                                                         0225
 91    FORMAT('C','SURFACE AREA PER UNIT VOLUME=',E10.4,' SQ.FT.PER CU.FT    0226
      1.')                                                                   0227
       WRITE(6,116) PCROS                                                    0228
116    FORMAT('C','POROSITY (VOLUME OF VOID PER UNIT VOLUME=',E10.4)         0229
       WRITE(6,92) PERM                                                      0230
 92    FORMAT('C','PERMIABILITY OF POROUS MEDIUM=',E10.4,' SQ.FT.')          0231
       WRITE(6,93) ZPORE                                                     0232
 93    FORMAT('C','NUMBER OF PORES PER SQ.FT.=',E10.4)                       0233
       WRITE(6,94) U2                                                        0234
 94    FORMAT('0','PORE VELOCITY=',E10.4,' FT. PER SEC.')                    0235
       WRITE(6,95) DEL1                                                      0236
 95    FORMAT('C','AVG. PORE DIAMETER=',E10.4,' INCHES')                     0237
       WRITE(6,96) ROA                                                       0238
```

```
 96     FORMAT('0','DENSITY OF AIR=',E10.4,' LBM PER CU.FT.')
        WRITE(6,98) ACOND
 98     FORMAT('0','CONDUCTIVITY OF AIR=',E10.4,' BTU PER FT*HR*DEG-F')
        WRITE(6,99) VISC
 99     FORMAT('0','VISCOSITY OF AIR=',E10.4,' LBM PER FT**2*HR')
        WRITE(6,100) COND
100     FORMAT('0','CONDUCTIVITY OF POROUS MEDIUM=',E10.4,' BTU PER FT*HR*
     XDEG-F')
        WRITE(6,102) RADCON
102     FORMAT('0','RADIATION COEF. OF MEDIUM FOR T-CUBED TERM=',E10.4,' B
     XTU PER FT*HR*DEG-F**4')
        WRITE(6,106) ROG1
106     FORMAT('0','DENSITY OF POROUS MEDIUM=',E10.4,' LBM PER CU.FT.')
        WRITE(6,108) RE
108     FORMAT('0','REYNOLDS NUMBER FOR EXTERIOR FLOW=',E10.4)
        WRITE(6,110) REIN
110     FORMAT('0','REYNOLDS NUMBER FOR INTERNAL FLOW=',E10.4)
        WRITE(6,112) CONV
112     FORMAT('0','INTERNAL CONVECTION HEAT TRANSFER COEF.=',E10.4,' BTU P
     XER SQ.FT*HR*DEG-F',/)
        WRITE(6,115)
115     FORMAT('0',3X,'THE FOLLOWING INTERNAL PROPERTIES WILL VARY WITH TE
     XMPERATURE:',/,5X,' 1.  PORE VELOCITY',/,5X,' 2.  DENSITY OF AIR',/
     X,5X,' 3.  CONDUCTIVITY OF AIR',/,5X,' 4.  INTERNAL CONVECTION HEAT
     X TRANSFER COEF.',/,5X,' 5.  VISCOSITY OF AIR',/,5X,' 6.  DIFFUSION
     X COEFFICIENT',/,5X,' 7.  CONDUCTIVITY OF POROUS MEDIUM')
C
C
C****  INITIAL CONDITIONS*****
C
        NNPA=3*NNP-2
        NNPB=NNPA+1
        NNPC=NNPA+2
        READ(5,125) (CHI(1,I),I=1,NNPA,3)
125     FORMAT(F12.7)
        READ(5,125) (CHI(1,I),I=2,NNPB,3)
        READ(5,125) (CHI(1,I),I=3,NNPC,3)
        WRITE(6,130)
130     FORMAT('0','INITIAL CONDITIONS:  NP     TEMP-G          TEMP-A
     X CONC-C2')
140     FORMAT(' ',21X,I2,3X,F7.2,7X,F7.2,8X,F7.5)
        NN=1
        DO 145 N=1,NNP
        NNN=NN+2
        WRITE(6,140) N,(CHI(1,I),I=NN,NNN)
        NN=NNN+1
145     CONTINUE
```

```
      DO 147 I=1,NNP
      III=3*I-2
      JJJ=III+1
      KKK=III+2
      Y1(I)=CHI(1,III)
      Y2(I)=CHI(1,JJJ)
      Y3(I)=CHI(1,KKK)
      X1(I)=X(I)
147   CONTINUE
C
C  LOCAL-GLOBAL CORRESPONDENCE****
C
      J=0
      DO 155 IEL=1,NEL
      DO 150 I=1,2
      ICOR(IEL,I)=J+1
      J=J+1
150   CONTINUE
      J=J-1
155   CONTINUE
      WRITE(6,160)
160   FORMAT('0','LOCAL-GLOBAL POINT CORRESPONDENCE')
      WRITE(6,165)
165   FORMAT('0',5X,'ELEM.    LNP1   LNP2   (GNP CORRESPONDENCE BELOW)')
      WRITE(6,170) (IEL,(ICOR(IEL,I),I=1,2),IEL=1,NEL)
170   FORMAT(' ',7X,I2,6X,I2,5X,I2)
CCCC
CC  NON-DIMENSIONALIZE I.C.****
C
      DO 190 I=1,NNPA,3
      CHI(1,I)=CHI(1,I)/TAPE
190   CONTINUE
      DO 195 I=2,NNPB,3
      CHI(1,I)=CHI(1,I)/TAPE
195   CONTINUE
      CAPB=FORCS*CAMB1
      DO 200 I=3,NNPC,3
      CHI(1,I)=CHI(1,I)/CAPB
200   CONTINUE
CCCC
CC  FORMATION OF PRELIMINARY SYSTEM MATRICES****
C
      CALL FORM1
C
```

```
C
CCC  SET COMBUSTION RATE PARAMETER****
C
      DO 202 NCHK=1,NAPC
      RACHK(NCHK)=ROG1
202   CONTINUE
CCC
CCC
CCC  PRINT BOUNDARY CONDITIONS****
C
      WRITE(6,225) HSURFL,EMIS
225   FORMAT('0','THE LEFT NATURAL B.C. FOR THE GRAPHITE ENERGY EQ.HAS A
     XS H-SURF.CONVECTION=',F6.2,' AND EMISSIVITY=',F4.2)
      WRITE(6,255) HSURFR,EMIS
255   FORMAT('0','THE RIGHT NATURAL B.C. FOR THE GRAPHITE ENERGY EQ. HAS
     X AS H-SURF.CONVECTION=',F6.2,' AND EMISSIVITY=',F4.2)
260   WRITE(6,270) TAMB
270   FORMAT('0','THE LEFT ESSENTIAL B.C. FOR THE AIR ENERGY EQ. IS: T=
     X',F6.2)
      WRITE(6,271)
271   FORMAT('0','THE RIGHT NATURAL B.C. FOR THE AIR ENERGY EQUATION IS:
     X  D(T-A)/D(X)=D(T-G)/D(X)')
      WRITE(6,273) CAMB
273   FORMAT('0','THE LEFT B.C. FOR THE O2-CONC EQ. IS: (DIFF)*D(CONC.)/
     XD(X)=U(1)*(CONC.(1)-',F6.4,'LBM PER FT**3)')
      WRITE(6,275)
275   FORMAT('0','THE RIGHT NATURAL B.C. FOR THE O2-CONC. EQ. IS: D(CONC
     X.)/D(X)=0.0'//)
280   FORMAT(' ','ER VARIABLE FROM DERVAL IN SOLVER ROUTINE:')
      WRITE(6,280)

C
CCC
CCC  INTEGRATION DO-LOOP****
C
      TIME=0.0
      TOLD=0.0
      TEND=0.0
      IJK=0
      NL=0
      JSKF=0
      MAXDER=6
      H=.1E-4
      HMIN=.1E-6
      RMSEPS=1.0E-3
```

```
500    IJK=IJK+1                                                              0383
       TEND=TEND+T                                                            0384
C                                                                             0385
C                                                                             0386
C     CALL FORM2****                                                          0387
C                                                                             0388
       CALL FORM2                                                             0389
C                                                                             0390
C                                                                             0391
C     COMBUSTION RATE CHECK****                                               0392
C                                                                             0393
       DELT=TIME-TOLD                                                         0394
       DO 282 NCHK=3,NNPC,3                                                   0395
       RACHK(NCHK)=RACHK(NCHK)-ZMASS(NCHK)*DELT                               0396
       IF(RACHK(NCHK).GT.0.0) GO TO 282                                       0397
       NSTOP=NNFC/3                                                           0398
       WRITE(6,283) NSTOP                                                     0399
283    FORMAT('0',/,'TERMINATION DUE TO TOTAL CONSUMPTION OF FIBER AT N.      0400
      XP.=',I2)                                                               0401
       GO TO 501                                                              0402
282    CONTINUE                                                               0403
       TOLD=TIME                                                              0404
C                                                                             0405
C                                                                             0406
C     BOUNDARY CONDITION ADJUSTMENT****                                       0407
C                                                                             0408
       FF1=XLENTH/COND2(1)*(HSURFL-EMIS*.1714E-08/TAMB*((459.7+TAMB*CHI       0409
      X(1,1))**4-(459.7+TAMB)**4))                                            0410
       F(1)=F(1)+FF1                                                          0411
       ZKADD1=-XLENTH/COND2(1)*HSURFL                                         0412
       ZK(1,1)=ZK(1,1)+ZKADD1                                                 0413
       F(NNFB)=0.0                                                            0414
       FF2=XLENTH/COND2(NEL)*(HSURFR-EMIS*.1714E-08/TAMB*((459.7+TAMB         0415
      X*CHI(1,NNFA))**4-(459.7+TAMB)**4))                                     0416
       F(NNFA)=F(NNFA)+FF2                                                    0417
       F(NNFB)=F(NNFA)                                                        0418
       F(3)=F(3)+U2(1)*XLENTH                                                 0419
       ZKADD2=-XLENTH/COND2(NEL)*HSURFR                                       0420
       ZK(NNFA,NNFA)=ZK(NNFA,NNFA)+ZKADD2                                     0421
       ZK(NNFB,NNFA)=ZK(NNFB,NNFA)+ZKADD2                                     0422
285    DO 286 I=1,NNPC                                                        0423
       ZK(2,I)=0.0                                                            0424
       ZDOT(2,I)=0.0                                                          0425
       ZDOT(1,I)=0.0                                                          0426
286    CONTINUE                                                               0427
```

```
      ZDOT(2,2)=1.0                                                          0431
      ZK(3,3)=ZK(3,3)-U2(1)*XLENTH                                           0432
C                                                                            0433
C                                                                            0434
CCCCC INTEGRATE ZDOT****                                                     0435
C                                                                            0436
      CALL SDESOL(CHI,YL,TIME,TEND,NNPC,NL,NNPC,JSKP,MAXDER,0,F,HMIN,HMA     0437
     X),RMSERR,6)                                                            0438
      DO 310 I=1,NNP                                                         0439
      II=3*I-2                                                               0440
      JJ=II+1                                                                0441
      KK=II+2                                                                0442
      C(II)=CHI(1,II)*TAME                                                   0443
      C(JJ)=CHI(1,JJ)*TAME                                                   0444
      IF(CHI(1,KK).LT.0.0) CHI(1,KK)=1.0E-12                                 0445
      C(KK)=CHI(1,KK)*CAME                                                   0446
      TABS=TAMB*CHI(1,II)*455.7                                              0447
      HGR(KK)=(1.0-POROS)*1408E.0*4.014E7*(2.0/D)*RGAS*(CHI(1,KK)*CAMB       0448
     X*TABS)**.5/(EXP(39EE.C/TABS)*(12.0**3))                                0449
310   CONTINUE                                                               0450
CCCCC                                                                        0451
CCCCC                                                                        0452
CCCCC BOUNDARY CONDITION ADJUSTMENT AFTER INTEGRATION****                    0453
C                                                                            0454
      ZK(1,1)=ZK(1,1)-ZKADD1                                                 0455
      ZK(NNPA,NNPA)=ZK(NNPA,NNPA)-ZKADD2                                     0456
      ZK(NNPB,NNPA)=ZK(NNPB,NNPA)-ZKADD2                                     0457
314   ZK(3,3)=ZK(3,3)+U2(1)*XLENTH                                           0458
CCCCC                                                                        0459
CCCCC                                                                        0460
CCCCC PRINT NEW CHI'S****                                                    0461
C                                                                            0462
      TIME2=TSTART+TIME                                                      0463
      WRITE(6,315) TIME2                                                     0464
315   FORMAT('0',/,' AT TIME=',F8.4,' SEC.',/)                               0465
      WRITE(6,320)                                                           0466
320   FORMAT(' ',' ',' NP TEMP-G TEMP-A CONC-O2                              0467
     X  H.C.F.(BTU PER CU.IN*HR)',/)                                         0468
330   FORMAT(' ',3X,I2,6X,F6.2,6X,F8.2,8X,F7.5,8X,F11.3)                     0469
      NN=1                                                                   0470
      DO 335 N=1,NNP                                                         0471
      NNN=NN+2                                                               0472
      WRITE(6,330) N,(C(I),I=NN,NNN),HGR(NNN)                                0473
      NN=NNN+1                                                               0474
335   CONTINUE                                                               0475
```

```
      DO 350 I=1,NNP                                                    0479
      III=3*I-2                                                         0480
      JJJ=III+1                                                         0481
      KKK=III+2                                                         0482
      Y1(I)=C(III)                                                      0483
      Y2(I)=C(JJJ)                                                      0484
      Y3(I)=C(KKK)                                                      0485
      IF(C(III).GT.2200.0) GO TO 501                                    0486
350   CONTINUE                                                          0487
      Y4(1)=TIME                                                        0488
      X2(1)=I                                                           0489
      IF(ABS(T(31)-TAMB).LT.1.0) GO TO 501                              0490
      IF(TIME.GT.500.0) GO TO 501                                       0491
      GO TO 500                                                         0492
501   STOP                                                              0493
      END                                                               0494
C                                                                       0495
CCCC                                                                    0496
CCCC                                                                    0497
CCCC                                                                    0498
C SUBROUTINE FORM1****                                                  0499
C                                                                       0500
      SUBROUTINE FORM1                                                  0501
      REAL*8 ZK,ZDOT                                                    0502
      COMMON ZK(75,75),ZDOT(75,75),XLENTH,COND,RADCON,CONV,Z,ROG,       0503
     XDELP,FORCE,CHI(7,75),TAMB,TAMB,F(75),                             0504
     XPAMB,ACACC(25,4),BDOT(25,4),BSH(25,4),X(75),L,CD(25,4),           0505
     XRGAS,BOFCC(25,4),CC(25,4),ADOT(25,4),BETA,GCOND,D,SPHTG,RCA,SPHTA,0506
     XCOND2(25),TORT,CC2(25,4),SPHT,ZMASS(75),PERM,VISC,                0507
     XU2(25),NNP,NNPA,NNPB,NNPC,NEL,ICOR(75,2),IJK                      0508
C                                                                       0509
CCCC                                                                    0510
C ZERO OUT THE MATRICES****                                             0511
C                                                                       0512
      IZ=3*NNP                                                          0513
      DO 110 I=1,IZ                                                     0514
      F(I)=0.0                                                          0515
      DO 100 J=1,IZ                                                     0516
      ZK(I,J)=0.0                                                       0517
      ZDOT(I,J)=0.0                                                     0518
100   CONTINUE                                                          0519
110   CONTINUE                                                          0520
C                                                                       0521
CCCC                                                                    0522
C FORM ELEMENTAL COEFFICIENTS****                                       0523
```

```
C
      DO 500 IEL=1,NEL                                                  0527
      IIEL=IEL+1                                                        0528
      II=ICOR(IEL,1)*3-2                                                0529
      JJ=ICOR(IEL,2)*3-2                                                0530
      KK=II+1                                                           0531
      LL=JJ+1                                                           0532
      MM=II+2                                                           0533
      NN=JJ+2                                                           0534
      ZL=X(IIEL)-X(IEL)                                                 0535
      AK11=1.0/ZL                                                       0536
      AK12=-AK11                                                        0537
      AK21=AK12                                                         0538
      AK22=AK11                                                         0539
      ACACC(IEL,1)=Z*ZL*XLENTH**2/(3.0*(1.0-PCROS))                     0540
      ACACC(IEL,2)=ACACC(IEL,1)/2.0                                     0541
      ACACC(IEL,3)=ACACC(IEL,2)                                         0542
      ACACC(IEL,4)=ACACC(IEL,1)                                         0543
      ADCT(IEL,1)=PCO*SPHTC*ZL/3.0*XLENTH**2*3600.0                     0544
      ADCT(IEL,2)=ADCT(IEL,1)/2.0                                       0545
      ADCT(IEL,3)=ADCT(IEL,2)                                           0546
      ADCT(IEL,4)=ADCT(IEL,1)                                           0547
      BK11=1.0/ZL                                                       0548
      BK12=-BK11                                                        0549
      BK21=BK12                                                         0550
      BK22=BK11                                                         0551
      BSH(IEL,1)=-.5*XLENTH*SPHTA                                       0552
      BSH(IEL,2)=-BSH(IEL,1)                                            0553
      BSH(IEL,3)=BSH(IEL,1)                                             0554
      BSH(IEL,4)=BSH(IEL,2)                                             0555
      BCBCC(IEL,1)=Z*ZL*XLENTH**2/(3.0*PCROS)                           0556
      BCBCC(IEL,2)=BCBCC(IEL,1)/2.0                                     0557
      BCBCC(IEL,3)=BCBCC(IEL,2)                                         0558
      BCBCC(IEL,4)=BCBCC(IEL,1)                                         0559
      BDCT(IEL,1)=XLENTH**2*ZL*SPHTA/3.0*3600.0                         0560
      BDCT(IEL,2)=BDCT(IEL,1)/2.0                                       0561
      BDOT(IEL,3)=BDOT(IEL,2)                                           0562
      BDCT(IEL,4)=BCCT(IEL,1)                                           0563
      CD(IEL,1)=1.0/(ZL*TCPT)                                           0564
      CD(IEL,2)=-CC(IEL,1)                                              0565
      CD(IEL,3)=CC(IEL,2)                                               0566
      CD(IEL,4)=CD(IEL,1)                                               0567
      CC(IEL,1)=-XLENTH/2.0                                             0568
      CC(IEL,2)=-CC(IEL,1)                                              0569
      CC(IEL,3)=CC(IEL,1)                                               0570
      CC(IEL,4)=CC(IEL,2)                                               0571
      CC2(IEL,1)=-(XLENTH*TAME)/3.0                                     0572
      CC2(IEL,2)=CC2(IEL,1)/2.0                                         0573
                                                                        0574
```

```
      CC2(IEL,3)=CC2(IEL,2)                                                    0575
      CC2(IEL,4)=CC2(IEL,1)                                                    0576
      CDCT11=(XLENTH**2)*2L/3.C*3600.0                                         0577
      CDCT12=CDCT11/2.0                                                        0578
      CDCT21=CDCT12                                                            0579
      CDCT22=CDCT11                                                            0580
C                                                                              0581
CCCCC                                                                          0582
CCCCC DISTRIBUTE ELEMENT COEFFICIENTS INTO SYSTEM MATRICES****                 0583
C                                                                              0584
      ZK(II,II)=ZK(II,II)-AK11                                                 0585
      ZK(II,JJ)=ZK(II,JJ)-AK12                                                 0586
      ZK(JJ,II)=ZK(JJ,II)-AK21                                                 0587
      ZK(JJ,JJ)=ZK(JJ,JJ)-AK22                                                 0588
      ZK(KK,KK)=ZK(KK,KK)-EK11                                                 0589
      ZK(KK,LL)=ZK(KK,LL)-EK12                                                 0590
      ZK(LL,KK)=ZK(LL,KK)-EK21                                                 0591
      ZK(LL,LL)=ZK(LL,LL)-EK22                                                 0592
      ZDCT(MM,MM)=ZDCT(MM,MM)+CDCT11                                           0593
      ZDCT(MM,NN)=ZDCT(MM,NN)+CDCT12                                           0594
      ZDCT(NN,MM)=ZDCT(NN,MM)+CDCT21                                           0595
      ZDCT(NN,NN)=ZDCT(NN,NN)+CDCT22                                           0596
500   CONTINUE                                                                 0597
      RETURN                                                                   0598
      END                                                                      0599
C                                                                              0600
CCCCC                                                                          0601
CCCCC                                                                          0602
CCCCC                                                                          0603
CCCCC SUBROUTINE FORM2****                                                     0604
C                                                                              0605
      SUBROUTINE FORM2                                                         0606
      REAL*8 ZK,ZDCT,GAMMA,GAM                                                 0607
      COMMON ZK(75,75),ZDCT(75,75),XLENTH,CONC,RADCON,CONV,Z,ROG,              0608
     XDELP,PCRCS,CHI(7,75),TAMB,CAMB,F(75),                                    0609
     XFAMB,ACACC(25,4),BDCT(25,4),BSH(25,4),X(75),U,CD(25,4),                  0610
     XRGAS,BCECC(25,4),CC(25,4),ADOT(25,4),BETA,GCOND,D,SPHTG,ROA,SPHTA,       0611
     XCOND2(25),TORT,CC2(25,4),SPHT,ZMASS(75),PERM,VISC,                       0612
     XU2(25),NNF,NNFA,NNPE,NNPC,NEL,ICOR(75,2),IJK                             0613
      DIMENSION TVGA(50),CONV2(25),ACOND2(25),ROA2(25),CONC2(25)               0614
      DO 2 IN1=1,NNPC                                                          0615
      F(IN1)=C.C                                                               0616
      ZMASS(IN1)=C.C                                                           0617
2     CONTINUE                                                                 0618
      DO 500 IEL=1,NEL                                                         0619
      II=ICOR(IEL,1)*3-2                                                       0620
```

```
      JJ=ICCR(IEL,2)*3-2                                                        0623
      KK=II+1                                                                   0624
      LL=JJ+1                                                                   0625
      MM=II+2                                                                   0626
      NN=JJ+2                                                                   0627
      IF(I.K.EC.1) GC TC 5                                                      0628
      ZDCT(II,II)=ZDOT(II,II)-ADCT(IEL,1)/CCNC2(IEL)                            0629
      ZDCT(II,JJ)=ZDOT(II,JJ)-ADOT(IEL,2)/COND2(IEL)                            0630
      ZDCT(JJ,II)=ZDCT(JJ,II)-ADOT(IEL,3)/CCNC2(IEL)                            0631
      ZDCT(JJ,JJ)=ZDOT(JJ,JJ)-ADOT(IEL,4)/CONC2(IEL)                            0632
      ZK(II,II)=ZK(II,II)+ACACC(IEL,1)*CONV2(IEL)/COND2(IEL)                    0633
      ZK(II,JJ)=ZK(II,JJ)+ACACC(IEL,2)*CONV2(IEL)/CCND2(IEL)                    0634
      ZK(JJ,II)=ZK(JJ,II)+ACACC(IEL,3)*CONV2(IEL)/CCND2(IEL)                    0635
      ZK(JJ,JJ)=ZK(JJ,JJ)+ACACC(IEL,4)*CONV2(IEL)/CONC2(IEL)                    0636
      ZK(II,KK)=ZK(II,KK)-ACACC(IEL,1)*CONV2(IEL)/CCND2(IEL)                    0637
      ZK(II,LL)=ZK(II,LL)-ACACC(IEL,2)*CONV2(IEL)/COND2(IEL)                    0638
      ZK(JJ,KK)=ZK(JJ,KK)-ACACC(IEL,3)*CONV2(IEL)/CCNC2(IEL)                    0639
      ZK(JJ,LL)=ZK(JJ,LL)-ACACC(IEL,4)*CONV2(IEL)/COND2(IEL)                    0640
      ZDCT(KK,KK)=ZDCT(KK,KK)-BCOT(IEL,1)/ACONC2(IEL)*ROA2(IEL)                 0641
      ZDCT(KK,LL)=ZDCT(KK,LL)-BCOT(IEL,2)/ACCNC2(IEL)*RCA2(IEL)                 0642
      ZDCT(LL,KK)=ZDOT(LL,KK)-BCOT(IEL,3)/ACONC2(IEL)*RCA2(IEL)                 0643
      ZDCT(LL,LL)=ZDCT(LL,LL)-BCOT(IEL,4)/ACOND2(IEL)*ROA2(IEL)                 0644
      ZK(KK,KK)=ZK(KK,KK)+BSH(IEL,1)*U2(IEL)*RCA2(IEL)/ACONC2(IEL)              0645
      ZK(KK,LL)=ZK(KK,LL)+BSH(IEL,2)*U2(IEL)*ROA2(IEL)/ACOND2(IEL)              0646
      ZK(LL,KK)=ZK(LL,KK)+BSH(IEL,3)*U2(IEL)*RCA2(IEL)/ACONC2(IEL)              0647
      ZK(LL,LL)=ZK(LL,LL)+BSH(IEL,4)*U2(IEL)*ROA2(IEL)/ACOND2(IEL)              0648
      ZK(KK,II)=ZK(KK,II)-BCBCC(IEL,1)*CONV2(IEL)/ACOND2(IEL)                   0649
      ZK(KK,JJ)=ZK(KK,JJ)-BCBCC(IEL,2)*CONV2(IEL)/ACOND2(IEL)                   0650
      ZK(LL,II)=ZK(LL,II)-BCBCC(IEL,3)*CONV2(IEL)/ACOND2(IEL)                   0651
      ZK(LL,JJ)=ZK(LL,JJ)-BCBCC(IEL,4)*CONV2(IEL)/ACONC2(IEL)                   0652
      ZK(KK,KK)=ZK(KK,KK)+BCBCC(IEL,1)*CONV2(IEL)/ACONC2(IEL)                   0653
      ZK(KK,LL)=ZK(KK,LL)+BCBCC(IEL,2)*CONV2(IEL)/ACOND2(IEL)                   0654
      ZK(LL,KK)=ZK(LL,KK)+BCBCC(IEL,3)*CONV2(IEL)/ACOND2(IEL)                   0655
      ZK(LL,LL)=ZK(LL,LL)+BCBCC(IEL,4)*CONV2(IEL)/ACOND2(IEL)                   0656
      ZK(MM,MM)=ZK(MM,MM)+CC(IEL,1)*TVGA(IEL)                                   0657
      ZK(MM,NN)=ZK(MM,NN)+CC(IEL,2)*TVGA(IEL)                                   0658
      ZK(NN,MM)=ZK(NN,MM)+CC(IEL,3)*TVGA(IEL)                                   0659
      ZK(NN,NN)=ZK(NN,NN)+CC(IEL,4)*TVGA(IEL)                                   0660
      ZK(MM,MM)=ZK(MM,MM)+CC(IEL,1)*U2(IEL)                                     0661
      ZK(MM,NN)=ZK(MM,NN)+CC(IEL,2)*U2(IEL)                                     0662
      ZK(NN,MM)=ZK(NN,MM)+CC(IEL,3)*U2(IEL)                                     0663
      ZK(NN,NN)=ZK(NN,NN)+CC(IEL,4)*U2(IEL)                                     0664
      ZK(MM,MM)=ZK(MM,MM)+CC2(IEL,1)*CONC2(IEL)                                 0665
      ZK(MM,NN)=ZK(MM,NN)+CC2(IEL,2)*CONC2(IEL)                                 0666
      ZK(NN,MM)=ZK(NN,MM)+CC2(IEL,3)*CONC2(IEL)                                 0667
      ZK(NN,NN)=ZK(NN,NN)+CC2(IEL,4)*CONC2(IEL)                                 0668
    5 IIEL=IEL+1                                                                0669
      ZL=X(IIEL)-X(IEL)                                                         0670
```

```
      TG=(CHI(1,II)+CHI(1,JJ))*TAMB/2.0                                  0671
      TA=(CHI(1,KK)+CHI(1,LL))*TAMB/2.0                                  0672
      TAVGG=TG+459.7                                                     0673
      TAVGA=TA+459.7                                                     0674
      VISC2=-1.041E-8*TA**2+6.02EEE-5*TA+.0354                           0675
      ACOND2(IEL)=-3.232E-8*TA**2+2.412E-5*TA+.0131                      0676
      RCA2(IEL)=PAMB/(RGAS*TAVGA)                                        0677
      L2(IEL)=RCA*L/RCA2(IEL)                                            0678
      G2=U2(IEL)*POROS*RCA2(IEL)                                         0679
      REIN=G2/(2*VISC2*.511)                                             0680
      CONV2(IEL)=.828*SPHT*G2/(REIN**.51*(SPHTA*VISC2/ACOND2(IEL))**.61) 0681
      ZKAPPA=ACOND2(IEL)/GCOND                                           0682
      GAMMA=(1.0/BETA)*ZKAPPA/(1.0-ZKAPPA)                               0683
      GAM=DSQRT(1.0-GAMMA*GAMMA)                                         0684
      GAMCHK=10.E-01                                                     0685
      IF(GAM.LT.GAMCHK) GO TO 6                                          0686
      PI1=DLOG((1.0D1-GAM)/GAMMA)                                        0687
      GM=1.0-GAMMA*GAMMA                                                 0688
      PI2=1.0+GAMMA/SQRT(GM)*PI1                                         0689
      COND2(IEL)=(ACOND2(IEL)/(1.0-BETA*PI2)+PACCOA*TAVGG**3)            0690
      LPRI=RCA*L*RGAS/PAMB                                               0691
      TVGA(IEL)=((TAVGA*.55)**1.5)*1.6754E-04                            0692
      COX2=(CHI(1,MM)+CHI(1,NN))/2.0                                     0693
      CCND2(IEL)=UPRI*(CHI(1,KK)-CHI(1,LL))                              0694
      RATE=(32.0/12.01)*4.0146E7*(2.0/D)*(COX2**.5)*RGAS*ZL*(XLENTH**2)* 0695
     X(TAVGG**.5)/(EXP(35883.0/TAVGG)*2.0*(CAMB**.5))                    0696
      RATEH=(12.0/32.0)*14085.0*RATE*CAMB/(CCND2(IEL)*TAMB)              0697
      CHECK=(12.0/32.0)*RATE*CAMB/(ZL*XLENTH**2*3600.0)                  0698
      ZDOT(II,II)=ZDOT(II,II)+ADOT(IEL,1)/CCND2(IEL)                     0699
      ZDOT(II,JJ)=ZDOT(II,JJ)+ADOT(IEL,2)/CCND2(IEL)                     070C
      ZDOT(JJ,II)=ZDOT(JJ,II)+ADOT(IEL,3)/CCND2(IEL)                     0701
      ZDOT(JJ,JJ)=ZDOT(JJ,JJ)+ADOT(IEL,4)/CCND2(IEL)                     0702
      ZK(II,II)=ZK(II,II)-ACACC(IEL,1)*CONV2(IEL)/CCND2(IEL)             0703
      ZK(II,JJ)=ZK(II,JJ)-ACACC(IEL,2)*CONV2(IEL)/CCND2(IEL)             0704
      ZK(JJ,II)=ZK(JJ,II)-ACACC(IEL,3)*CONV2(IEL)/CCND2(IEL)             0705
      ZK(JJ,JJ)=ZK(JJ,JJ)-ACACC(IEL,4)*CONV2(IEL)/CCND2(IEL)             0706
      ZK(II,KK)=ZK(II,KK)+ACACC(IEL,1)*CONV2(IEL)/CCND2(IEL)             0707
      ZK(II,LL)=ZK(II,LL)+ACACC(IEL,2)*CONV2(IEL)/CCND2(IEL)             0708
      ZK(JJ,KK)=ZK(JJ,KK)+ACACC(IEL,3)*CONV2(IEL)/CCND2(IEL)             0709
      ZK(JJ,LL)=ZK(JJ,LL)+ACACC(IEL,4)*CONV2(IEL)/CCND2(IEL)             071C
      ZDOT(KK,KK)=ZDOT(KK,KK)+BDOT(IEL,1)/ACCND2(IEL)*RCA2(IEL)          0711
      ZDOT(KK,LL)=ZDOT(KK,LL)+BDOT(IEL,2)/ACCND2(IEL)*RCA2(IEL)          0712
      ZDOT(LL,KK)=ZDOT(LL,KK)+BDOT(IEL,3)/ACCND2(IEL)*RCA2(IEL)          0713
      ZDOT(LL,LL)=ZDOT(LL,LL)+BDOT(IEL,4)/ACCND2(IEL)*RCA2(IEL)          0714
      ZK(KK,KK)=ZK(KK,KK)-BSH(IEL,1)*U2(IEL)*RCA2(IEL)/ACOND2(IEL)       0715
      ZK(KK,LL)=ZK(KK,LL)-BSH(IEL,2)*U2(IEL)*RCA2(IEL)/ACOND2(IEL)       0716
      ZK(LL,KK)=ZK(LL,KK)-BSH(IEL,3)*U2(IEL)*RCA2(IEL)/ACOND2(IEL)       0717
      ZK(LL,LL)=ZK(LL,LL)-BSH(IEL,4)*U2(IEL)*RCA2(IEL)/ACOND2(IEL)       071E
    6 PI1=DLOG((1.0D1-GAM)/GAMMA)
```

```
      ZK(KK,II)=ZK(KK,II)+BCBCC(IEL,1)*CONV2(IEL)/ACONC2(IEL)                    0719
      ZK(KK,JJ)=ZK(KK,JJ)+BCBCC(IEL,2)*CONV2(IEL)/ACOND2(IEL)                   0720
      ZK(LL,II)=ZK(LL,II)+BCBCC(IEL,3)*CONV2(IEL)/ACOND2(IEL)                   0721
      ZK(LL,JJ)=ZK(LL,JJ)+BCBCC(IEL,4)*CONV2(IEL)/ACOND2(IEL)                   0722
      ZK(KK,KK)=ZK(KK,KK)-BCBCC(IEL,1)*CONV2(IEL)/ACOND2(IEL)                   0723
      ZK(KK,LL)=ZK(KK,LL)-BCBCC(IEL,2)*CONV2(IEL)/ACOND2(IEL)                   0724
      ZK(LL,KK)=ZK(LL,KK)-BCBCC(IEL,3)*CONV2(IEL)/ACOND2(IEL)                   0725
      ZK(LL,LL)=ZK(LL,LL)-BCBCC(IEL,4)*CONV2(IEL)/ACONC2(IEL)                   0726
      ZK(MM,MP)=ZK(MM,MM)-CD(IEL,1)*TVGA(IEL)                                   0727
      ZK(MP,NP)=ZK(MP,NN)-CD(IEL,2)*TVGA(IEL)                                   0728
      ZK(NN,MP)=ZK(NN,MP)-CD(IEL,3)*TVGA(IEL)                                   0729
      ZK(NN,NN)=ZK(NN,NN)-CD(IEL,4)*TVGA(IEL)                                   0730
      ZK(MP,MP)=ZK(MP,MM)-CC(IEL,1)*U2(IEL)                                     0731
      ZK(MM,NN)=ZK(MM,NN)-CC(IEL,2)*U2(IEL)                                     0732
      ZK(NN,MP)=ZK(NN,MM)-CC(IEL,3)*U2(IEL)                                     0733
      ZK(NN,NN)=ZK(NN,NN)-CC(IEL,4)*U2(IEL)                                     0734
      ZK(MM,MP)=ZK(MM,MM)-CC2(IEL,1)*CONC2(IEL)                                 0735
      ZK(MP,NN)=ZK(MP,NN)-CC2(IEL,2)*CONC2(IEL)                                 0736
      ZK(NN,MP)=ZK(NN,MP)-CC2(IEL,3)*CONC2(IEL)                                 0737
      ZK(NN,NN)=ZK(NN,NN)-CC2(IEL,4)*CONC2(IEL)                                 0738
      F(II)=F(II)+RATEH                                                         0739
      F(JJ)=F(JJ)+RATEH                                                         0740
      F(MM)=F(MM)-RATE                                                          0741
      F(NN)=F(NN)-RATE                                                          0742
      ZMASS(MP)=ZMASS(MM)+CHECK                                                 0743
      ZMASS(NP)=ZMASS(NN)+CHECK                                                 0744
500   CONTINUE                                                                  0745
      ZMASS(3)=2.0*ZMASS(3)                                                     0746
      ZMASS(NNFC)=2.0*ZMASS(NNFC)                                               0747
      RETURN                                                                    0748
      END                                                                       0749
C                                                                               0750
C                                                                               0751
C                                                                               0752
C                                                                               0753
C                                                                               0754
C  SUBROUTINE DIFFUN****                                                        0755
C                                                                               0756
      SUBROUTINE DIFFUN(Y,YL,T,HINV,DY)                                         0757
      REAL*8 ZK,ZDOT                                                            0758
      COMMON ZK(75,75),ZDOT(75,75),XLENTH,CONC,RADCON,CONV,Z,ROG,               0759
     XCELP,PCRCS,CHI(7,75),TAMB,CAMB,F(75),                                     0760
     XFAMB,ACACC(25,4),BCCT(25,4),BSH(25,4),X(75),U,CD(25,4),                   0761
     XRGAS,BCECC(25,4),CC(25,4),ACCT(25,4),BETA,GCOND,D,SPHTG,ROA,SPHTA,        0762
     XCOND2(25),TORT,CC2(25,4),SPHT,ZMASS(75),PERM,VISC,                        0763
     XU2(25),NNF,NNFA,NNFE,NNFC,NEL,ICOR(75,2),IJK                              0764
      DIMENSION Y(7,1),YL(1),DY(1)                                              0765
      IA=1                                                                      0766
```

```
      IB=3                                                              0767
      JA=1                                                              0768
      JB=6                                                              0769
      DO 300 K=1,NAP                                                    0770
      DO 200 I=IA,IB                                                    0771
      DY(I)=0.0                                                         0772
      DO 100 J=JA,JB                                                    0773
      DY(I)=DY(I)+ZDOT(I,J)*Y(2,J)*HINV-ZK(I,J)*Y(1,J)                  0774
  100 CONTINUE                                                          0775
      DY(I)=DY(I)-F(I)                                                  0776
  200 CONTINUE                                                          0777
      IA=IA+3                                                           0778
      IB=IB+3                                                           0779
      IF(K.EQ.1) GO TO 5                                                0780
      JA=JA+3                                                           0781
      IF(K.EQ.NEL) GO TO 300                                            0782
    5 JB=JB+3                                                           0783
  300 CONTINUE                                                          0784
      RETURN                                                            0785
      END                                                               0786
C                                                                       0787
CCCCCC                                                                  0788
                                                                        0789
CCCCCC                                                                  0790
C     SUBROUTINE JACMAT****                                             0791
C                                                                       0792
      SUBROUTINE JACMAT(Y,YL,T,HINV,A2,N,NY,EPS,DY,F1,PW)               0793
      REAL*8 ZK,ZDOT                                                    0794
      COMMON ZK(75,75),ZDOT(75,75),XLENTH,COND,RADCON,CONV,Z,RCG,       0795
     XDELP,FCFCS,CHI(7,75),TAMB,CAMB,F(75),                             0796
     XFAMB,ACACC(25,4),BDOT(25,4),BSH(25,4),X(75),U,CD(25,4),           0797
     XRGAS,BCBCC(25,4),CC(25,4),ACOT(25,4),BETA,GCCND,C,SPHTG,RCA,SPHTA,0798
     XCCND2(25),TORT,CC2(25,4),SPHT,ZMASS(75),PERM,VISC,                0799
     XU2(25),NAF,NAPA,NAPB,NAPC,NEL,ICOR(75,2),IJK                      0800
      DIMENSION Y(7,1),YL(1),F1(1),DY(1),PW(N,1)                        0801
      AH=-A2*HINV                                                       0802
      DO 75 I=1,N                                                       0803
      DO 50 J=1,N                                                       0804
      PW(I,J)=0.0                                                       0805
   50 CONTINUE                                                          0806
   75 CONTINUE                                                          0807
      IA=1                                                              0808
      IB=3                                                              0809
      JA=1                                                              0810
      JB=6                                                              0811
      DO 300 K=1,NAP                                                    0812
      DO 200 I=IA,IB                                                    0813
      DO 100 J=JA,JB                                                    0814
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```
      FW(I,J)=AH*ZDOT(I,J)-ZK(I,J)                                      0815
100   CONTINUE                                                          0816
200   CONTINUE                                                          0817
      IA=IA+3                                                           0818
      IB=IB+3                                                           0819
      IF(K.EQ.J) GO TO 5                                                0820
      JA=JA+3                                                           0821
      IF(K.EQ.NEL) GO TO 300                                            0822
5     JB=JB+3                                                           0823
300   CONTINUE                                                          0824
      RETURN                                                            0825
      END                                                               0826
C                                                                       0827
C                                                                       0828
      SUBROUTINE SDESCL (Y,YL,T,TEND,NY,NL,M,JSKF,MAXDER,IPRT,H,HMIN,   0829
     1HMAX,RMSEPS,W)                                                    0830
C     ------------------------------------------------------------------0831
C                                                                       0832
C     SUBROUTINE SDESCL IS A DRIVER ROUTINE FOR SUBROUTINE LDASUB.      0833
C     ITS PURPOSE IS TO SET UP THE NECESSARY REFERENCES TO A LARGE      0834
C     BLOCK OF AUXILLARY STORAGE, AND  OBTAIN INITIAL VALUES OF         0835
C     DERIVATIVES.                                                      0836
C     THE CALLING SEQUENCE FOR SDESCL IS                                0837
C                                                                       0838
C CALL SDESCL(Y,YL,T,TEND,NY,NL,M,JSKF,MAXDER,IPRT,H,HMIN,HMAX,RMSEPS,W)0839
C                                                                       0840
C     WHERE THE PARAMETERS ARE DEFINED AS FOLLOWS.                      0841
C                                                                       0842
C        Y       - ARRAY DIMENSIONED (7,NY).  THIS ARRAY CONTAINS THE   0843
C                  DEPENDENT VARIABLES AND THEIR SCALED DERIVATIVES.    0844
C                  Y(J+1,I) CONTAINS THE J-TH DERIVATIVE OF THE I-TH VAR0845
C                  IABLE TIMES H**J/J-FACTORIAL, WHERE H IS THE CURRENT 0846
C                  STEPSIZE.  ON FIRST ENTRY THE CALLER SUPPLIES THE    0847
C                  INITIAL VALUES OF EACH VARIABLE IN Y(1,I).  ON SUB-  0848
C                  SEQUENT ENTRIES IT IS ASSUMED THE ARRAY HAS NOT      0849
C                  BEEN CHANGED.  TO INTERPOLATE TO NON-MESH POINTS,    0850
C                  THESE VALUES CAN BE USED AS FOLLOWS.  IF H IS THE    0851
C                  CURRENT STEPSIZE AND VALUES AT TIME  T+E  ARE        0852
C                  NEEDED, LET  S = E/H  AND THEN                       0853
C                                                                       0854
C                                                    JS                 0855
C                       I-TH VARIABLE AT  T+E IS   SUM Y(J+1,I)*S**J    0856
C                                                  J=0                  0857
C                                                                       0858
C                  THE VALUE OF JS IS OBTAINED IN THE CALLING PROGRAM   0859
C                  BY  JS = IABS(JSKF/10)                               0860
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C     YL      - ARRAY OF NL VARIABLES WHICH APPEAR LINEARLY.                  0863
C     T       - CURRENT VALUE OF THE INDEPENDENT VARIABLE (TIME)              0864
C     TEND    - END TIME                                                      0865
C     NY      - NUMBER OF DIFFERENTIAL EQUATIONS AND NONLINEAR                0866
C               VARIABLES.                                                    0867
C     NL      - NUMBER OF LINEAR VARIABLES                                    0868
C     M       - NUMBER OF VARIABLES INCLUDED IN THE ERROR TEST                0869
C     JSKF    - AN INDICATOR USED BOTH ON INPUT AND OUTPUT                    0870
C               ON INPUT, JSKF = -1 INDICATES A RESTART CALL TO               0871
C               SDESOL.  JSKF = 0 INDICATES AN INITIAL CALL TO                0872
C               SDESOL.  JSKF > 0 INDICATES A CONTINUATION OF THE             0873
C               PREVIOUS CALL TO SDESOL.  JSKF < -1 MAY HAVE RESULTED         0874
C               FROM THE USER NEGLECTING TO TEST FOR ERROR RETURNS            0875
C               FROM SDESOL.  BECAUSE OF THIS POSSIBILITY, JSKF < -1          0876
C               RESULTS IN TERMINATION OF THE RUN WITH THE                    0877
C               APPROPRIATE COMMENT.                                          0878
C               ON OUTPUT, JSKF CONSISTS OF TWO DIGITS AND SIGN,              0879
C               + CR - OF.  Q IS THE ORDER OF THE FORMULA CURRENTLY           0880
C               BEING USED.  P INDICATES THE TYPE OF RETURN, AS               0881
C               FOLLOWS.                                                      0882
C               JSKF > 0, P = 1 IS THE NORMAL RETURN                          0883
C               JSKF < 0 IS AN ERROR RETURN, WITH THE FOLLOWING               0884
C               MEANINGS.                                                     0885
C                    P = 1  ERROR TEST FAILURE FOR H > HMIN                   0886
C                    P = 3  CORRECTOR FAILED TO CONVERGE FOR H > HMIN         0887
C                    P = 4  CORRECTOR FAILED TO CONVERGE FOR FIRST            0888
C                           ORDER METHOD                                      0889
C                    P = 5  ERROR RETURN FROM SUBROUTINE NUITSL               0890
C                    P = 6  ERROR RETURN FROM SUBROUTINE DERVAL               0891
C     MAXDER  - MAXIMUM ORDER DERIVATIVE THAT SHOULD BE USED IN               0892
C               METHOD.  IT MUST BE NO GREATER THAN SIX.                      0893
C     IPRT    - INTERNAL PRINT CONTROL INDICATOR FOR LDASUB.                  0894
C                    IPRT = 0  NO PRINT                                       0895
C                    IPRT > 0  PRINT COUNTERS, STEPSIZE, CURRENT TIME         0896
C                              AND VALUES OF DEPENDENT VARIABLES AT           0897
C                              EACH STEP.                                     0898
C     H       - CURRENT STEPSIZE.  AN INITIAL VALUE MUST BE SUPPLIED          0899
C               BUT NEED NOT BE THE ONE WHICH MUST BE USED, SINCE THE         0900
C               SUBROUTINE WILL CHOSE A SMALLER ONE IF NECCESSARY TO          0901
C               KEEP THE ERROR PER STEP SMALLER THAN THE SPECIFIED            0902
C               VALUE.  IT IS BETTER TO UNDERESTIMATE THE INITIAL             0903
C               STEPSIZE THAN TO OVERESTIMATE IT.  THE STEPSIZE IS            0904
C               NORMALLY NOT CHANGED BY THE USER.                             0905
C     HMIN    - MINIMUM STEPSIZE ALLOWED                                      0906
C     HMAX    - MAXIMUM STEPSIZE ALLOWED                                      0907
C     RPSEPS  - THE ERROR TEST CONSTANT.  THE ROOT-MEAN-SQUARE OF             0908
C               THE SINGLE STEP ERROR ESTIMATES, ER(I), DIVIDED BY            0909
C               YMAX(I) = (MAXIMUM TO CURRENT TIME OF Y(I) ) MUST BE          0910
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C                 LESS THAN EPS.  THE STEPSIZE AND/OR THE ORDER                  0911
C                 ARE VARIED TO ACHIEVE THIS.                                    0912
C        W      - SCRATCH STORAGE ARRAY.  MUST BE AT LEAST 13*NY + 5*NL          0913
C                 LOCATIONS, PLUS THOSE REQUIRED FOR STORAGE OF THE              0914
C                 MATRIX  PW (SEE DESCRIPTION OF SUBROUTINE JACMAT).             0915
C                 THE STORAGE OF PW WILL NORMALLY REQUIRE NO MORE THAN           0916
C                 N**2 + 2*N LOCATIONS, AND IF COMPACT STORAGE TECH-             0917
C                 NIQUES ARE USED, CAN BE MUCH FEWER.                            0918
C                                                                                0919
C     ------------------------------------------------------------------         0920
      DIMENSION Y(7,1), YL(1), W(1)                                              0921
      IF (JSKF.GT.0) GO TO 120                                                   0922
      IF (JSKF.LT.-1) GO TO 140                                                  0923
      N = NY*NL                                                                  0924
      IF (JSKF.LT.0) GO TO 110                                                   0925
C                                                                                0926
C     IF THIS IS THE FIRST ENTRY, OBTAIN VALUES OF THE DERIVATIVES.              0927
      CALL DERVAL (Y,YL,T,N,NY,W,KRETR)                                          0928
      IF (KRETR.NE.0) GO TO 130                                                  0925
C                                                                                0930
C     NOW SET UP STORAGE BLOCKS IN THE W ARRAY.  THIS NEEDS TO BE DONE           0931
C     ONLY INITIALLY AND ON RESTARTS.                                            0932
C                                                                                0933
C        THE ARRAY   SAVE    STARTS AT LOCATION  1      IN THE W ARRAY         0934
C        THE ARRAY   YLSV    STARTS AT LOCATION  NSVL   IN THE W ARRAY         0935
C        THE ARRAY   YMAX    STARTS AT LOCATION  NYMAX  IN THE W ARRAY         0936
C        THE ARRAY   ER      STARTS AT LOCATION  NER    IN THE W ARRAY         0937
C        THE ARRAY   ESV     STARTS AT LOCATION  NESV   IN THE W ARRAY         0938
C        THE ARRAY   F1      STARTS AT LOCATION  NF1    IN THE W ARRAY         0939
C        THE ARRAY   DY      STARTS AT LOCATION  NDY    IN THE W ARRAY         0940
C        THE MATRIX  PW      STARTS AT LOCATION  NPW    IN THE W ARRAY         0941
C                                                                                0942
  110 NSVL = 7*NY+1                                                              0943
      NYMAX = NSVL+NL                                                            0944
      NER = NYMAX+NY                                                             0945
      NESV = NER+NY                                                              0946
      NF1 = NESV+NY                                                              0947
      NDY = NF1+N                                                                0948
      NPW = NDY+N                                                                0949
  120 JS = JSKF                                                                  0950
      CALL LCASUB (Y,YL,T,TEND,N,NY,M,JS,KF,MAXDER,IPRT,H,HMIN,HMAX,             0951
     1RMSERS,W,W(NSVL),W(NYMAX),W(NER),W(NESV),W(NF1),W(NDY),W(NPW))             0952
C                                                                                0953
C     CODE JSKF ON RETURN FROM LCASUB                                            0954
C                                                                                0955
      JSKF = ISIGN(JS*IC+IABS(KF),KF)                                            0956
      RETURN                                                                     0957
  130 JSKF = -6                                                                  0958
```

```
      RETURN                                                            0959
  140 PRINT 1, JSKF                                                     0960
      STOP                                                              0961
C                                                                       0962
C                                                                       0963
    1 FORMAT ('0IT IS AN ERROR TO ENTER SDESCL WITH JSKF = ',I10//      0964
     1 '    RUN HAS BEEN TERMINATED.')                                  0965
      END                                                               0966
      SUBROUTINE LCASUB (Y,YL,T,TEND,N,NY,M,JSTART,KFLAG,MAXOR,IPRT,H,  0967
     1HMIN,HMAX,RNSEPS,SAVE,YLSV,YMAX,ER,ESV,F1,DY,PW)                  0968
C                                                                       0969
C     WHICH IS DUE TO R. L. BROWN AND C. W. GEAR.  DFASUB IS DOCUMENTED 0970
C     IN THE REPORT                                                     0971
C        DOCUMENTATION FOR DFASUB--                                     0972
C        BY R. L. BROWN AND C. W. GEAR                                  0973
C        REPORT UIUCDCS-R-73-575, JULY 1973                             0974
C        UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN                     0975
C        URBANA, ILLINOIS  61801                                        0976
C     THIS REPORT IS AVAILABLE FROM THE NATIONAL TECHNICAL INFORMATION  0977
C     SERVICE OF THE U. S. DEPARTMENT OF COMMERCE UNDER ACCESSION NUMBER 0978
C     COM-1469-225.                                                     0979
C                                                                       0980
C     THE MODIFICATION HERE IS DOCUMENTED IN THE REPORT                 0981
C        A PROGRAM FOR THE NUMERICAL SOLUTION OF LARGE SPARSE SYSTEMS OF 0982
C        ALGEBRAIC AND IMPLICITLY DEFINED STIFF DIFFERENTIAL EQUATIONS  0983
C        BY RICHARD FRANKE                                              0984
C        REPORT NPS53FE76051, MAY 1976                                  0985
C        NAVAL POSTGRADUATE SCHOOL                                      0986
C        MONTEREY, CALIFORNIA  93940                                    0987
C                                                                       0988
C     ------------------------------------------------------------------0989
C                                                                       0990
C     THE CALLING SEQUENCE FOR LCASUB IS                                0991
C                                                                       0992
C     CALL LCASUB(Y,YL,T,TEND,N,NY,M,JSTART,KFLAG,MAXOR,IPRT,H,HMIN,    0993
C     HMAX,RNSEPS,SAVE,YLSV,YMAX,ER,ESV,F1,DY,PW)                       0994
C                                                                       0995
C     WHERE THE PARAMETERS ARE DEFINED AS FOLLOWS.                      0996
C        Y        - ARRAY DIMENSIONED (7,NY).  THIS ARRAY CONTAINS THE  0997
C                   DEPENDENT VARIABLES AND THEIR SCALED DERIVATIVES.   0998
C                   Y(J+1,I) CONTAINS THE J-TH DERIVATIVE OF THE I-TH VAR 0999
C                   IABLE TIMES H**J/J-FACTORIAL, WHERE H IS THE CURRENT 1000
C                   STEPSIZE.  ON FIRST ENTRY THE CALLER SUPPLIES THE   1001
C                   INITIAL VALUES OF EACH VARIABLE IN Y(1,I) AND AN    1002
C                   ESTIMATE OF THE INITIAL VALUES OF THE DERIVATIVES   1003
C                   IN Y(2,I).  ON SUBSEQUENT ENTRIES IT IS ASSUMED THAT 1004
C                   THE ARRAY HAS NOT BEEN CHANGED.  TO INTERPOLATE TO  1005
C                   NON-MESH POINTS, THESE VALUES CAN BE USED AS FOLLOWS. 1006
```

```
C
C                IF H IS THE CURRENT STEPSIZE AND VALUES AT TIME T+E          1007
C                NEEDED, LET S = E/H  AND THEN                                1008
C                                                                             1009
C                                                  NC                         1010
C                     I-TH VARIABLE AT  T+E IS   SUM Y(J+1,I)*S**J            1011
C                                                J=0                          1012
C                                                                             1013
C                THE VALUE OF NC IS OBTAINED IN THE CALLING PROGRAM           1014
C                BY  NC = JSTART.                                             1015
C                                                                             1016
C       YL       - ARRAY OF NL = N - NY VARIABLES WHICH APPEAR LINEARLY.      1017
C                  THE USER SUPPLIES INITIAL VALUES FOR THESE VARIABLES.      1018
C       T        - CURRENT VALUE OF THE INDEPENDENT VARIABLE (TIME)           1019
C       TEND     - END TIME                                                   1020
C       N        - TOTAL NUMBER OF VARIABLES                                  1021
C       NY       - NUMBER OF DIFFERENTIAL EQUATIONS AND NONLINEAR             1022
C                  VARIABLES.                                                 1023
C       M        - NUMBER OF VARIABLES INCLUDED IN THE ERROR TEST.            1024
C                  THIS NUMBER CAN BE NO GREATER THAN NY.  IF IT IS           1025
C                  GREATER THAN NY, NY VARIABLES ARE USED IN THE ERROR        1026
C                  TEST.                                                      1027
C       JSTART   - INPUT AND OUTPUT INDICATOR.                                1028
C                  ON INPUT JSTART HAS THE FOLLOWING MEANINGS.                1029
C                       <0  THIS INDICATES A RE-START FROM A PREVIOUS         1030
C                           POINT FOLLOWING TERMINATION OF THE RUN OR         1031
C                           SOLUTION OF ANOTHER PROBLEM DURING THE SAME       1032
C                           RUN.  PARAMETERS IN THE CALLING SEQUENCE          1033
C                           MUST HAVE BEEN PRESERVED FROM THE PREVIOUS        1034
C                           USE, PARTICULARLY THE ARRAYS                      1035
C                              SAVE, YLSV, ESV, AND PW.                       1036
C                           THESE ARRAYS MUST BE SAVED AFTER A CALL           1037
C                           TO SUBROUTINE LDASAV, WHICH ALSO SAVES            1038
C                           NECESSARY PARAMETERS INTERNAL TO LDASUB.          1039
C                       =0  INDICATES AN INITIAL CALL TO LDASUB.  THE         1040
C                           ROUTINE INITIALIZES ITSELF, SCALES THE            1041
C                           DERIVATIVES IN Y(2,I) AND THEN PERFORMS THE       1042
C                           INTEGRATION UNTIL T > TEND.                       1043
C                       >0  INDICATES THE SOLUTION IS TO BE CONTINUED.        1044
C                           AFTER THE INITIAL ENTRY IT IS NEITHER             1045
C                           DESIRABLE NOR NECESSARY TO RE-ENTER WITH          1046
C                           JSTART = 0, SINCE THIS RE-INITIALIZES             1047
C                           THE CODE, BEGINNING WITH A FIRST ORDER            1048
C                           METHOD AGAIN.                                     1049
C                  ON OUTPUT, JSTART IS SET TO THE VALUE OF NC, THE           1050
C                  ORDER OF THE FORMULA CURRENTLY BEING USED.                 1051
C       KFLAG    - THE COMPLETION CODE INDICATOR, WITH THE FOLLOWING          1052
C                  MEANINGS                                                   1053
C                       +1  THE INTEGRATION WAS SUCCESSFUL                    1054
```

```
C                      -1  ERROR TEST FAILURE FOR H > HMIN                      1055
C                      -2  CORRECTOR FAILED TO CONVERGE FOR H > HMIN            1056
C                      -4  CORRECTOR FAILED TO CONVERGE FOR FIRST               1057
C                          ORDER METHOD                                         1058
C                      -5  ERROR RETURN FROM SUBROUTINE NUITSL                  1059
C        MAXCR    - MAXIMUM ORDER DERIVATIVE THAT SHOULD BE USED IN THE        1060
C                   METHOD.  IT MUST BE NO GREATER THAN SIX.  IF IT IS         1061
C                   GREATER THAN SIX, THE MAXIMUM ORDER USED WILL BE SIX.      1062
C        IPRT     - INTERNAL PRINT CONTROL INDICATOR                           1063
C                      = 0  NO PRINT                                           1064
C                      > 0  PRINT COUNTERS, STEPSIZE, CURRENT TIME             1065
C                           AND VALUES OF DEPENDENT VARIABLES AT               1066
C                           EACH STEP.                                         1067
C        H        - CURRENT STEPSIZE.  AN INITIAL VALUE MUST BE SUPPLIED       1068
C                   BUT NEED NOT BE THE ONE WHICH WILL BE USED, SINCE THE      1069
C                   SUBROUTINE WILL CHOOSE A SMALLER ONE IF NECCESSARY TO      1070
C                   KEEP THE ERROR PER STEP SMALLER THAN THE SPECIFIED         1071
C                   VALUE.  IT IS BETTER TO UNDERESTIMATE THE INITIAL          1072
C                   STEPSIZE THAN TO OVERESTIMATE IT.  THE STEPSIZE IS         1073
C                   NORMALLY NOT CHANGED BY THE USER.                          1074
C        HMIN     - MINIMUM STEPSIZE ALLOWED                                   1075
C        HMAX     - MAXIMUM STEPSIZE ALLOWED                                   1076
C        RPSERS   - THE ERROR TEST CONSTANT.  THE ROOT-MEAN-SQUARE OF          1077
C                   THE SINGLE STEP ERROR ESTIMATES, ER(I), DIVIDED BY         1078
C                   YMAX(I) * (MAXIMUM TO CURRENT TIME OF Y(I)) MUST BE        1079
C                   LESS THAN RPSERS.  THE STEPSIZE AND/OR ORDER ARE           1080
C                   VARIED TO ACHIEVE THIS.                                    1081
C        SAVE     - AN ARRAY OF LENGTH AT LEAST 7*NY                           1082
C        YLSV     - AN ARRAY OF LENGTH AT LEAST NL                             1083
C        YMAX     - A VECTOR OF LENGTH NY WHICH CONTAINS THE MAXIMUM           1084
C                   OF EACH Y SEEN SO FAR.  ON THE FIRST CALL, THESE WILL      1085
C                   BE INITIALIZED AS YMAX(I) = MAX(1,|Y(1,I)|)                1086
C        ER       - A VECTOR OF LENGTH NY                                      1087
C        ESV      - A VECTOR OF LENGTH NY                                      1088
C        FI       - A VECTOR OF LENGTH N = NY + NL                             1089
C        DY       - A VECTOR OF LENGTH N = NY + NL                             1090
C        PW       - AN ARRAY IN WHICH THE  J  MATRIX COMPUTED                  1091
C                   IN SUBROUTINE JACMAT WILL BE STORED.  SIZE WHICH           1092
C                   MUST BE ALLOWED IS DETERMINED BY THE STORAGE TECH-         1093
C                   NIQUE USED FOR IT, BUT NORMALLY WON'T BE MORE THAN         1094
C                   N**2 + 2*N LOCATIONS, THE LATTER 2*N BEING REQUIRED        1095
C                   BY THE LINEAR EQUATION SOLVER.                             1096
C                                                                              1097
C     ------------------------------------------------------------             1098
      DIMENSION Y(7,1), YL(1), SAVE(7,1), YMAX(1), ER(1), YLSV(1), FI(1)       1099
     1, PERT(6,3), COF(21), ESV(1), DY(1), PW(1), SAV(1), A(29)                1100
      EQUIVALENCE (A(8),ENC), (A(9),BR), (A(10),E), (A(11),EDWN),              1101
     1(A(12),ENC1), (A(13),ENC2), (A(14),ENC3), (A(15),EPS), (A(16),EUP)       1102
```

```
     2,(A(17),HNEW), (A(18),PEPSH), (A(19),IDCUB), (A(20),IWEVAL),
     3(A(21),K), (A(22),LCCPYL), (A(23),LCOPYY), (A(24),MAXDER),
     4(A(25),M1), (A(26),NL), (A(27),NQ), (A(28),NS), (A(29),NW)
C
C    ------------------------------------------------------------------
C
C    THE COEFFICIENTS IN THE PERT ARRAY ARE USED FOR ERROR TESTING AND
C    CHANGING STEPSIZE AND NEED TO BE ACCURATE TO ONLY A FEW DIGITS.
C
C    ------------------------------------------------------------------
     DATA PERT/4.,9.,16.,25.,36.,49.,9.,16.,25.,36.,49.,64.,1.,1.,.25,
    12.7oESE-2,1.7056SE-3,6.83929E-5/
C    ------------------------------------------------------------------
C
C    THE ENTRIES IN THE CCF ARRAY ARE THE COEFFICIENTS FOR THE STIFFLY
C    STABLE METHODS USED IN THIS PROGRAM AND ARE TO BE THE MACHINE
C    PRECISION EQUIVALENTS OF THE FOLLOWING CONSTANTS.
C
C    -1
C    -3/2 , -1/2
C    -11/6 , -1 , -1/6
C    -25/12 , -35/24 , -5/12 , -1/24
C    -137/60 , -15/8 , -17/24 , -1/8 , -1/120
C    -147/60 , -203/90 , -49/48 , -35/144 , -7/240 , -1/720
C
C    ------------------------------------------------------------------
     DATA CCF/-1.,-1.5,-.5,-1.833333,-1.,-.1666667,-2.083333,-1.458333,
    1-.4166667,-.04166667,-2.283333,-1.875,-.7083333,-.125,-.0083333333,
    2-2.45,-2.225556,-1.027833,-.2430556,-.02916667,-.001388889/
     IF (JSTART) 100,110,150
C    ------------------------------------------------------------------
C    IF THIS IS A RESTART ENTRY, RESTORE Y AND YL FROM THE SAVE AND
C    YLSV ARRAYS, WHERE THEY WERE SAVED BY A PREVIOUS CALL TO LDASAV.
C    ------------------------------------------------------------------
C
C
  100 CALL CCPYZ (Y,SAVE,LCCPYY)
     CALL CCPYZ (YL,YLSV,LCCPYL)
     GO TO 15C
C    ------------------------------------------------------------------
C    IF THIS IS THE FIRST CALL, INITIALIZE YMAX, SCALE DERIVATIVES, AND
C    INITIALIZE INDICATORS AND SET ORDER TO ONE.
C    FOR DOUBLE PRECISION, SET LCOPYL = 14*NY AND LCOPYL = 2*NL IF
C    SUBROUTINE CCPYZ IS IN SINGLE PRECISION.
C    ------------------------------------------------------------------
C
  110 NL = N-NY
     LCCPYY = 7*NY
     LCCPYL = NL
     M1 = MIN0(N,NY)
     EPS = SQRT(FLOAT(M1))*RMSEPS
```

```
      MAXCEF = MINO(MAXCF,6)                                                    1151
      IF (IPRT.LE.0) GO TO 120                                                  1152
      PRINT 3, N,NL,RMSEPS,TEND,H                                               1153
      PRINT 4                                                                   1154
  120 NS = 0                                                                    1155
      NW = 0                                                                    1156
C                                                                               1157
      DO 130 J=1,NY                                                             1158
      YMAX(J) = AMAX1(1.,ABS(Y(1,J)))                                           1159
  130 Y(2,J) = Y(2,J)*H                                                         1160
C                                                                               1161
      NC = 1                                                                    1162
      ER = 1.                                                                   1163
      ASSIGN 190 TO IRET                                                        1164
C     ------------------------------------------------------------------        1165
CCC   SET COEFFICIENTS FOR THE ORDER CURRENTLY BEING USED.                      1166
CCC   E IS A TEST FOR ERRORS OF THE CURRENT ORDER NQ                            1167
CCC   EUP IS TO TEST FOR INCREASING THE ORDER, EDWN FOR DECREASING THE          1168
CCC   ORDER.                                                                    1169
C     ------------------------------------------------------------------        1170
  140 K = NC*(NC-1)/2                                                           1171
      CALL COPY2 (A(2),COF(K+1),NQ)                                             1172
      K = NC+1                                                                  1173
      IDCUB = NC                                                                1174
      ENC1 = .5/NC                                                              1175
      ENC2 = .5/K                                                               1176
      ENQ3 = .5/(NQ+2)                                                          1177
      EPSQ = EPS**2                                                             1178
      E = PERT(NC,1)*EPSQ                                                       1179
      EUP = PERT(NQ,2)*EPSQ                                                     1180
      EDWN = PERT(NC,3)*EPSQ                                                    1181
      BND = (EPS*ENQ3)**2                                                       1182
      IWEVAL = 1                                                                1183
      GO TO IRET, (190,200,490,570)                                             1184
  150 IF (H.EQ.HNEW) GO TO 190                                                  1185
C     ------------------------------------------------------------------        1186
CCC   IF CALLER HAS CHANGED H, RESCALE DERIVATIVES TO REFLECT THAT HNEW         1187
CCC   WAS USED ON THE LAST CALL.                                                1188
C     ------------------------------------------------------------------        1189
      R = H/HNEW                                                                1190
      ASSIGN 190 TO IRET                                                        1191
      GO TO 610                                                                 1192
C     ------------------------------------------------------------------        1193
CCC   SET JSTART TO NQ, THE CURRENT ORDER OF THE METHOD, BEFORE EXIT,           1194
CCC   AND SAVE THE CURRENT STEPSIZE IN HNEW.                                    1195
C     ------------------------------------------------------------------        1196
  160 JSTART = NC                                                               1197
      HNEW = H                                                                  1198
```

```
      RETURN                                                            1199
  170 NS = NS+1                                                         1200
      IF (IPRT.LE.0) GO TO 180                                          1201
C     ------------------------------------------------------------------1202
C     PRINT DATA IF DESIRED BY USER                                     1203
C     ------------------------------------------------------------------1204
      PRINT 1, NS,NW,NQ,H,T,(Y(1,I),I=1,NY)                             1205
      IF (NL.GT.0) PRINT 2, (YL(I),I=1,NL)                              1206
  180 CONTINUE                                                          1207
      IF (KFLAG.LT.0) GO TO 160                                         1208
      IF (T.GE.TEND) GO TO 190                                          1209
C     ------------------------------------------------------------------1210
C     TAKE ANOTHER STEP IF T < TEND                                     1211
C     ------------------------------------------------------------------1212
      JSTART = 1                                                        1213
C     ------------------------------------------------------------------1214
C     SAVE DATA FOR TRIAL WITH A SMALLER TIMESTEP IF THIS STEP FAILS    1215
C     ------------------------------------------------------------------1216
  190 CALL COPYZ (SAVE,Y,LCOPYY)                                        1217
      CALL COPYZ (YLSV,YL,LCOPYL)                                       1218
      RACUM = 1.                                                        1219
      KFLAG = 1                                                         1220
      HOLD = H                                                          1221
      NQOLD = NQ                                                        1222
      TOLD = T                                                          1223
  200 T = T+H                                                           1224
      HINV = 1./H                                                       1225
C     ------------------------------------------------------------------1226
C     COMPUTE PREDICTED VALUES BY EFFECTIVELY MULTIPLYING DERIVATIVE    1227
C     VECTOR BY PASCAL TRIANGLE MATRIX                                  1228
C     ------------------------------------------------------------------1229
C                                                                       1230
      DO 210 J=2,K                                                      1231
      J3 = K+J-1                                                        1232
C                                                                       1233
      DO 210 J1=J,K                                                     1234
      J2 = J3-J1                                                        1235
C                                                                       1236
      DO 210 I=1,NY                                                     1237
  210 Y(J2,I) = Y(J2,I)+Y(J2+1,I)                                       1238
C                                                                       1239
      DO 220 I=1,NY                                                     1240
  220 ER(I) = 0.                                                        1241
C                                                                       1242
C     ------------------------------------------------------------------1243
C     GO UP TO THREE CORRECTOR ITERATIONS.  CONVERGENCE IS OBTAINED WHEN1244
C     CHANGES ARE LESS THAN ENC WHICH IS DEPENDENT ON THE ERROR TEST    1245
C                                                                       1246
```

```
C     CONSTANT.  THE SUM OF CORRECTIONS IS ACCUMULATED IN ER(I).  IT IS
C     EQUAL TO THE K-TH DERIVATIVE OF Y TIMES H**K/(K-FACTORIAL*A(K)),
C     AND THUS IS PROPORTIONAL TO THE ACTUAL ERRORS TO THE LOWEST POWER
C     OF H PRESENT, WHICH IS H**K.
C     ------------------------------------------------------------------
C
      DO 270 L=1,3
      CALL DIFFUN (Y,YL,T,HINV,DY)
      IF (IWEVAL.LT.1) GO TO 230
C     ------------------------------------------------------------------
C     IF THERE HAS BEEN A CHANGE OF ORDER OR THERE HAS BEEN TROUBLE
C     WITH CONVERGENCE, PW IS RE-EVALUATED PRIOR TO STARTING THE
C     CORRECTOR ITERATION.  IWEVAL IS THEN SET TO -1 AS AN INDICATOR
C     THAT IT HAS BEEN DONE.  NEWPW IS SET NONZERO TO INDICATE TO
C     SUBROUTINE NUITSL THAT A NEW PW HAS BEEN PROVIDED.
C     ------------------------------------------------------------------
      CALL JACMAT (Y,YL,T,HINV,A(2),N,NY,EPS,DY,F1,PW)
      KFLAG = 1
      IWEVAL = -1
      NW = NW+1
      NEWPW = 1
  220 CALL NLITSL (PW,DY,F1,N,NY,EPS,YMAX,NEWPW,KFRET)
      IF (KFRET.NE.0) GO TO 600
      IF (NL.LE.0) GO TO 250
C
      DO 240 I=1,NL
  240 YL(I) = YL(I)-F1(I+NY)
C
  250 CONTINUE
      DEL = 0.
C
      DO 260 I=1,NY
      Y(1,I) = Y(1,I)-F1(I)
      Y(2,I) = Y(2,I)+A(2)*F1(I)
      ER(I) = ER(I)+F1(I)
      DEL = DEL+(F1(I)/AMAX1(YMAX(I),ABS(Y(1,I))))**2
  260 CONTINUE
C
      IF (L.GE.2) BR = AMAX1(.5*ER,DEL/DEL1)
      DEL1 = DEL
      IF (AMIN1(DEL,ER*DEL*2.).LE.ENE) GO TO 330
  270 CONTINUE
C     ------------------------------------------------------------------
C     THE CORRECTOR ITERATION FAILED TO CONVERGE IN 3 TRIES.  VARIOUS
C     POSSIBILITIES ARE CHECKED FOR.  IF H IS ALREADY HMIN AND PW HAS
C     ALREADY BEEN RE-EVALUATED, A NO CONVERGENCE EXIT IS TAKEN.
C     OTHERWISE THE MATRIX PW IS RE-EVALUATED AND/OR (IN THAT ORDER) THE
```

```
C     STEP IS REDUCED TO TRY AND GET CONVERGENCE.                       1295
C     ------------------------------------------------------------------1296
      T = TOLD                                                          1297
      IF (INEVAL) 280,300,290                                           1298
  280 IF (H.LE.HMIN*1.0001) GO TO 310                                   1299
  290 RACUM = RACUM*.25                                                 1300
  300 CONTINUE                                                          1301
      GO TO 320                                                         1302
  310 KFLAG = -3                                                        1303
C     ------------------------------------------------------------------1304
C     RESTORE Y AND YL AFTER CONVERGENCE FAILURE                        1305
C     ------------------------------------------------------------------1306
  320 CALL COPYZ (Y,SAVE,LCOPYY)                                        1307
      CALL COPYZ (YL,YLSV,LCOPYL)                                       1308
      H = HOLD                                                          1309
      NQ = NQOLD                                                        1310
      GO TO 170                                                         1311
C     ------------------------------------------------------------------1312
C     THE CORRECTOR CONVERGED, SO NOW THE ERROR TEST IS MADE.           1313
C     ------------------------------------------------------------------1314
  330 D = 0.                                                            1315
C                                                                       1316
      DO 340 I=1,N1                                                     1317
      YM = AMAX1(ABS(Y(1,I)),YMAX(I))                                   1318
  340 D = D+(ER(I)/YM)**2                                               1319
C                                                                       1320
      INEVAL = 0                                                        1321
      IF (D.GT.E) GO TO 280                                             1322
C     ------------------------------------------------------------------1323
C     THE ERROR TEST IS OKAY, SO THE STEP IS ACCEPTED.  IF IDOLB        1324
C     NOW BECOMES NEGATIVE, A TEST IS MADE TO SEE IF THE STEP SIZE      1325
C     CAN BE INCREASED AT THIS ORDER OR ONE HIGHER OR ONE LOWER.        1326
C     THE CHANGE IS MADE ONLY IF THE STEP CAN BE INCREASED BY AT        1327
C     LEAST 10%.  IDOUB IS SET TO NQ TO PREVENT FURTHER TESTING         1328
C     FOR A WHILE.  IF NO CHANGE IS MADE, IDOLB IS SET TO 9.            1329
C     ------------------------------------------------------------------1330
      IF (K.LT.3) GO TO 360                                             1331
C                                                                       1332
      DO 350 J=3,K                                                      1333
C                                                                       1334
      DO 350 I=1,NY                                                     1335
  350 Y(J,I) = Y(J,I)+A(J)*ER(I)                                        1336
C                                                                       1337
  360 KFLAG = 1                                                         1338
      IDOLB = IDOLB-1                                                   1339
      IF (ICOLE) 410,370,510                                            1340
  370 CALL COPYZ (ESV,ER,N1)                                            1341
      GO TO 510                                                         1342
```

```
C     ------------------------------------------------------------------
CCC   THE ERROR TEST FAILED.  IF JSTART = 0, THE DERIVATIVES IN THE
CCC   SAVE ARRAY ARE UPDATED.  TESTS ARE THEN MADE TO FIX THE STEPSIZE
CCC   AND PERHAPS REDUCE THE ORDER.  AFTER RESTORING AND SCALING THE
CCC   Y VARIABLES, THE STEP IS RETRIED.
C     ------------------------------------------------------------------
  380 IF (JSTART.GT.0) GO TO 400
C
      DO 390 I=1,NY
  390 SAVE(2,I) = Y(2,I)
C
  400 KFLAG = KFLAG-2
      IF (P.LE.PMIN) GO TO 550
      T = TOLD
      IF (KFLAG.LE.-5) GO TO 530
  410 PR2 = (D/E)**ENQ2*1.2
      L = 0
      IF (NC.LE.1) GO TO 430
      D = 0.
C
      DO 420 J=1,M1
      YM = AMAX1(ABS(Y(1,J)),YMAX(J))
  420 D = D+(Y(K,J)/YM)**2
C
      PR1 = (D/EDWN)**ENC1*1.3
      IF (PR1.GE.PR2) GO TO 430
      PR2 = PR1
      L = -1
  430 IF (KFLAG.LT.0.OR.NC.GE.MAXDER) GO TO 450
      D = 0
C
      DO 440 J=1,M1
      YM = AMAX1(ABS(Y(1,J)),YMAX(J))
  440 D = D+((ER(J)-ESV(J))/YM)**2
C
      PR1 = (D/ELP)**ENC3*1.4
      IF (PR1.GE.PR2) GO TO 450
      PR2 = PR1
      L = 1
  450 R = 1./AMAX1(PR2,1.E-5)
      IF (KFLAG.LT.0.OR.R.GE.1.1) GO TO 460
      IDCUP = 5
      GO TO 510
  460 NEWC = NC+L
      K = NEWC+1
      IF (NEWC.LE.NC) GO TO 480
      R1 = A(NEWC)/FLOAT(NEWC)
C
```

```
      DO 470 J=1,NY                                                     1391
  470 Y(K,J) = ER(J)*R1                                                 1392
C                                                                       1393
  480 CONTINUE                                                          1394
CCC   ------------------------------------------------------------------1395
CCC   IF THE STEP WAS OKAY, SCALE THE Y VARIABLES IN ACCORDANCE         1396
CCC   WITH THE NEW VALUE OF H.  IF KFLAG < 0, HOWEVER, USE THE         1397
CCC   SAVED VALUES (IN SAVE AND YLSV).  IN EITHER CASE, IF THE ORDER    1398
CCC   HAS CHANGED IT IS NECESSARY TO FIX CERTAIN PARAMETERS BY CALLING  1399
CCC   THE PROGRAM SEGMENT AT STATEMENT NUMBER 140.                      1400
CCC   ------------------------------------------------------------------1401
      IDOUB = NQ                                                        1402
      IF (NEWQ.EQ.NQ) GO TO 490                                         1403
      NQ = NEWQ                                                         1404
      ASSIGN 490 TO IRET                                                1405
      GO TO 140                                                         1406
  490 IF (KFLAG.GT.0) GO TO 500                                         1407
      RACLM = RACLM*R                                                   1408
      GO TO 560                                                         1409
  500 R = AMAX1(AMIN1(HMAX/H,R),HMIN/H)                                 1410
      H = H*R                                                           1411
      IWEVAL = 1                                                        1412
      ASSIGN 510 TO IRET                                                1413
      GO TO 610                                                         1414
C                                                                       1415
  510 DO 520 I=1,N1                                                     1416
  520 YMAX(I) = AMAX1(ABS(Y(1,I)),YMAX(I))                              1417
C                                                                       1418
      GO TO 170                                                         1419
CCC   ------------------------------------------------------------------1420
CCC   THE ERROR TEST HAS NOW FAILED THREE TIMES, SO THE DERIVATIVES ARE 1421
CCC   IN BAD SHAPE.  RETURN TO FIRST ORDER METHOD AND TRY AGAIN.  OF    1422
CCC   COURSE, IF NQ = 1 ALREADY, THEN THERE IS NO HOPE AND WE EXIT WITH 1423
CCC   KFLAG = -4.                                                       1424
CCC   ------------------------------------------------------------------1425
  530 IF (NQ.EQ.1) GO TO 540                                            1426
      NQ = 1                                                            1427
      IDOUB = 1                                                         1428
      ASSIGN 570 TO IRET                                                1429
      GO TO 140                                                         1430
  540 NQOLD = 1                                                         1431
      KFLAG = -4                                                        1432
      GO TO 560                                                         1433
  550 KFLAG = -1                                                        1434
      GO TO 170                                                         1435
CCC   ------------------------------------------------------------------1436
CCC   THIS SECTION RESTORES THE SAVED VALUES OF Y AND YL, SCALING THE   1437
CCC   Y DERIVATIVES AS NECESSARY, AND THEN RETURNS TO THE PREDICTOR LOOP 1438
```

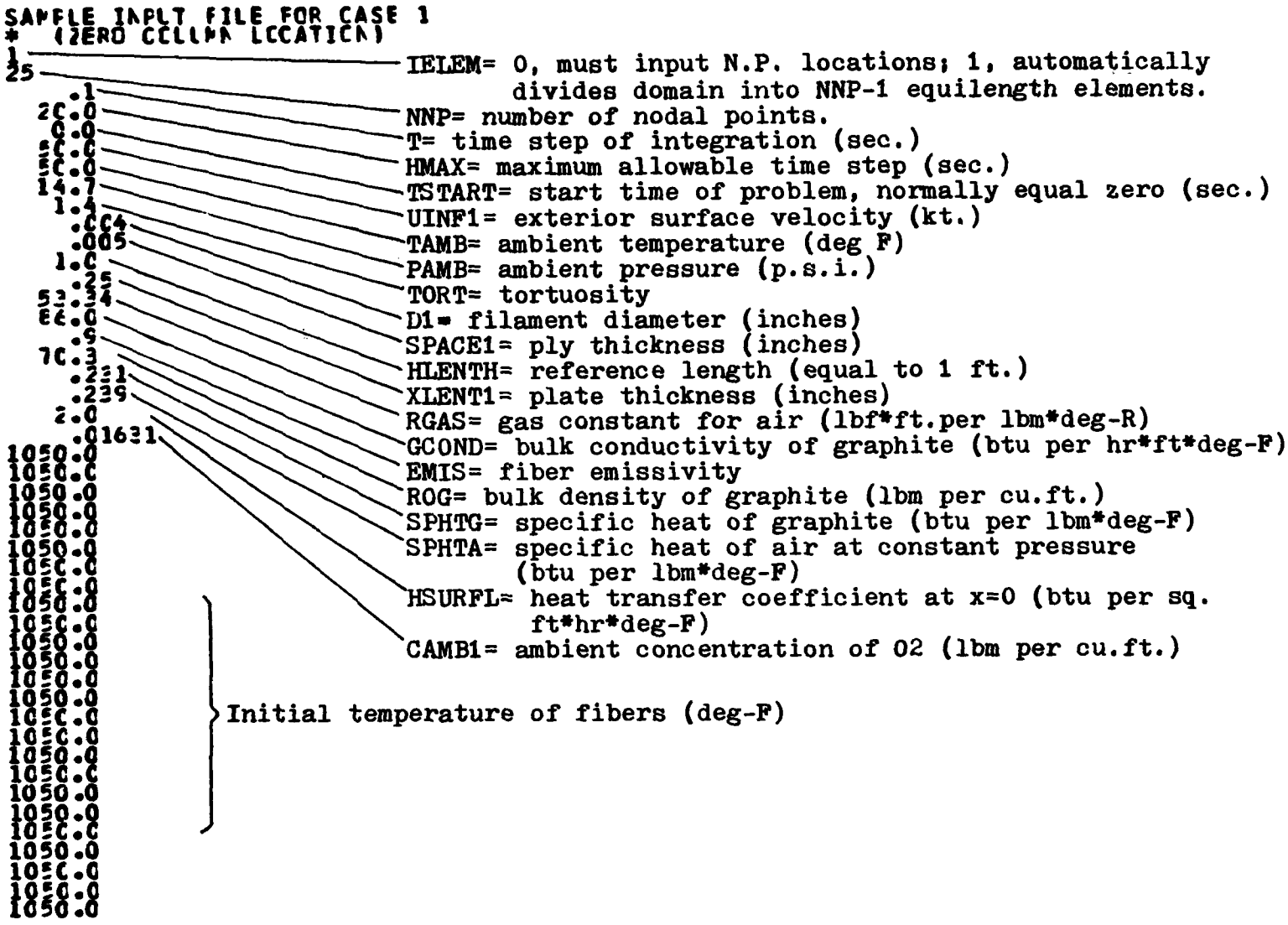
```
C     ------------------------------------------------------------------
  560 H = HCLC*RACUM                                                    1440
      H = AMAX1(HMIN,AMIN1(H,HMAX))                                     1441
  570 RACUM = H/HCLC                                                    1442
      R1 = 1.                                                           1443
C                                                                       1444
      DO 580 J=2,K                                                      1445
      R1 = R1*RACUM                                                     1446
C                                                                       1447
      DO 580 I=1,NY                                                     1448
  580 Y(J,I) = SAVE(J,I)*R1                                             1449
C                                                                       1450
CC                                                                      1451
      DO 590 I=1,NY                                                     1452
  590 Y(1,I) = SAVE(1,I)                                                1453
C                                                                       1454
      CALL CCPYZ (YL,YLSV,LCCPYL)                                       1455
      IWEVAL = 1                                                        1456
      GO TO 200                                                         1457
  600 KFLAG = -5                                                        1458
      GO TO 160                                                         1459
C     ------------------------------------------------------------------1460
CCC   THIS SECTION SCALES THE Y DERIVATIVES BY R**J                     1461
CCC   ------------------------------------------------------------------1462
  610 R1 = 1.                                                           1463
C                                                                       1464
      DO 620 J=2,K                                                      1465
      R1 = R1*R                                                         1466
C                                                                       1467
      DO 620 I=1,NY                                                     1468
  620 Y(J,I) = Y(J,I)*R1                                                1469
C                                                                       1470
      GO TO IRET, (190,510)                                             1471
C     ------------------------------------------------------------------1472
CCCCC THIS SECTION ALLOWS FOR RESTARTS AFTER SOLVING ANOTHER PROBLEM, OR 1473
CCCCC HAVING TERMINATED THE CURRENT COMPUTER RUN.  SUBROUTINE LDASAV     1474
CCCCC SAVES THE NECESSARY VALUES WHICH ARE INTERNAL TO LDASUB.  FOR      1475
CCCCC DOUBLE PRECISION, WITH CCPYZ IN SINGLE PRECISION, THE NUMBER OF   1476
CCCCC LOCATIONS TO BE SAVED AND RESTORED, LCOPYS AND LCCPYR, MUST BE     1477
CCCCC SET TO 88.                                                        1478
CCCCC IT IS ASSUMED THAT IN ADDITION TO THE VARIABLES IN THE ARRAY A     1479
CCCCC SAVED BY CALLING LDASAV, THE USER ALSO SAVES THE ARRAYS SAVE,      1480
CCCCC YLSV, YMAX, ESV, AND EWT.                                         1481
CCCCC                                                                   1482
CCCCC TO RESTART THE USER FIRST CALLS LDARST TO RESTORE THE VALUES SAVED 1483
CCCCC BY LDASAV, THEN RE-ENTERS LDASUB WITH JSTART < 0, AND WITH THE     1484
CCCCC OTHER PARAMETERS THE SAME AS RETURNED FROM THE LAST ENTRY TO       1485
C     LDASUB, PARTICULARLY THOSE ARRAYS MENTIONED ABOVE.                1486
```

```
C     ------------------------------------------------------------------
      ENTRY LCASAV(SAV)
      LCCPYS = 25
      CALL CCPYZ (SAV,A,LCCPYS)
      CALL CCPYZ (SAVE,Y,LCCPYY)
      CALL CCPYZ (YLSV,YL,LCCPYL)
      RETURN
C
      ENTRY LCARST(SAV)
      LCCPYR = 25
      CALL CCPYZ (A,SAV,LCCPYR)
      RETURN
CCCC  ------------------------------------------------------------------
CCCC
    1 FORMAT (2I5,I2,1P2E10.2,7E14.6/(32X,7E14.6))
    2 FORMAT (32X,1P7E14.6)
    3 FORMAT ('1  N =',I3,'   NL =',I3,'   RMSEPS =',1PE8.2,'   TEND ='
     1  ,E8.2,'   H =',E8.2//)
    4 FORMAT ('   NS   NW C    H',8X,'T   ',8X,'Y(1,*) AND YL(*)'//)
      END
      SUBROUTINE CCPYZ(S,Y,L)
      DIMENSION S(1),Y(1)
C     ------------------------------------------------------------------
CCCCC
CCCCC THIS SUBROUTINE COPIES THE ARRAY Y, OF LENGTH L, INTO THE ARRAY S
CCCCC
C     ------------------------------------------------------------------
      IF(L.LE.0)RETURN
      DO 100 J=1,L
  100 S(J) = Y(J)
      RETURN
      END
      SUBROUTINE DERVAL (Y,YL,T,N,NY,W,KERET)
C
CCCCC THIS SUBROUTINE CALCULATES THE INTIAL VALUES OF THE DERIVATIVES
CCCCC IN THE GENERAL CASE.  IT IS WRITTEN SO THAT IT SHOULD WORK IF THE
CCCCC FIRST NY EQUATIONS ALL INVOLVE DERIVATIVES.  IT ATTEMPTS TO SOLVE
CCCCC THE FIRST NY EQUATIONS USING NEWTON'S METHOD, BUT SINCE IT TRIES
CCCCC TO EVALUATE DF/DY' BY CALLING JACMAT IN SUCH A WAY AS TO MAKE THE
CCCCC DF/DY TERM INSIGNIFICANT, IT IS POSSIBLE THAT IT MAY FAIL FOR THAT
CCCCC REASON.  IT MAY FAIL FOR OTHER REASONS, AS WELL.  IF IT DOES FAIL
CCCCC THE USER CAN SUPPLY HIS OWN VERSION OF DERVAL, OR MODIFY THIS
CCCCC ROUTINE IN SUITABLE FASHION.  THIS ROUTINE ASSUMES THAT VALUES OF
CCCCC THE LINEAR VARIABLES HAVE BEEN SUPPLIED PREVIOUSLY.  IF THESE
CCCCC MUST BE SOLVED FOR SIMULTANEOUSLY WITH THE DERIVATIVES, THE USER
CCCCC MUST SUPPLY HIS OWN VERSION OF DERVAL.
```

```
C
C     THE CALLING SEQUENCE FOR THIS SUBROUTINE IS
C
C     CALL DERVAL(Y,YL,T,N,NY,W,KERET)
C
C     WHERE THE PARAMETERS ARE DEFINED AS FOLLOWS
C
C        Y        - SAME AS IN LDASUB AND SDESCL.  Y(1,I) CONTAINS THE
C                   INITIAL VALUES OF THE DEPENDENT VARIABLES.  THE
C                   VALUES OF THE DERIVATIVES ARE RETURNED IN Y(2,I).
C        YL       - SAME AS IN LDASUB AND SDESCL.  THE INITIAL VALUES OF
C                   THE LINEAR VARIABLES MUST BE SUPPLIED TO THIS VERSION
C        T        - INITIAL TIME
C        N        - SAME AS IN LDASUB, TOTAL NUMBER OF VARIABLES
C        NY       - SAME AS IN LDASUB, NUMBER OF DIFFERENTIAL EQUATIONS
C                   AND NONLINEAR VARIABLES
C        W        - SCRATCH ARRAY W FROM THE CALLING SEQUENCE OF SDESOL.
C                   THIS CAN BE USED AS NEEDED IN THIS SUBROUTINE.
C        KERET    - RETURN INDICATOR
C                      =0  NORMAL RETURN
C                      =1  ERROR RETURN
C
C     ------------------------------------------------------------------
      DIMENSION Y(2,1), YL(1), W(1)
C
      DO 100 I=1,NY
      W(2*N+I) = AMAX1(ABS(Y(1,I)),1.)
  100 Y(2,I) = 0.
C
      HINV = 10.**20
      KERET = 0
      EPS2 = NY*1.E6
      EPS = SQRT(EPS2)
C
      DO 140 IT=1,5
C
      DO 110 I=1,NY
  110 Y(2,I) = Y(2,I)/HINV
C
      CALL DIFFUN (Y,YL,T,HINV,W)
      CALL JACMAT (Y,YL,T,HINV,-1.,NY,NY,EPS,W,W(N+1),W(2*N+1))
      NEWPW = 1
C
      DO 120 I=1,NY
  120 W(I) = W(I)*HINV
C
      CALL ALITSL (W(2*N+1),W,W(N+1),NY,NY,EPS,W(2*N+1),NEWPW,KRET)
      IF (KRET.NE.0) GO TO 170
```

```
      ER = 0.
C
      DO 130 I=1,NY
      Y(3,I) = Y(3,I)-W(N+I)
  130 ER = ER+((W(N+I)/ANA)/(AMAX1(ABS(Y(3,I)),1.1))**2
      WRITE(6,131) ER
  131 FORMAT(2X,E12.5)
C
      IF (ER.LT.EPS2) GO TO 150
  140 CONTINUE
C
C     GO TO 170
C
  150 DO 160 I=1,NY
  160 Y(2,I) = Y(3,I)
C
      RETURN
  170 KERET = 1
      RETURN
      END
      SUBROUTINE NUITSL (PW,DY,F1,N,NY,EPS,YMAX,NEWPW,KRET)
C     ------------------------------------------------------------------
C
C     THE PURPOSE OF THIS SUBROUTINE IS TO SOLVE A
C     LINEAR SYSTEM OF EQUATIONS FOR THE NEWTON ITERATES WHEN THE
C     CORRECTOR EQUATION IS BEING SOLVED.  UPON ENTRY TO THIS SUBROUTINE
C     THE SYSTEM OF EQUATIONS TO BE SOLVED IS   J W = -F  , WHERE
C        J   IS STORED IN PW UPON ENTRY
C        W   IS RETURNED IN F1
C        -F  IS STORED IN DY UPON ENTRY
C
C     THIS SUBROUTINE IS GENERALLY SUPPLIED BY THE USER, ALTHOUGH THERE
C     ARE SOME STANDARD FORMS AVAILABLE.  FOR EXAMPLE, THIS VERSION
C     ASSUMES THAT PW IS STORED IN FULL STORAGE MODE IN AN NXN MATRIX.
C     IF NEWPW = 1, AN LU DECOMPOSITION IS DONE, NEWPW IS SET TO ZERO
C     AND FORWARD AND BACKWARD SUBSTITUTION FOR THE SOLUTION IS DONE.
C     IF NEWPW = 0, ONLY FORWARD AND BACKWARD SUBSTITUTION FOR THE
C     SOLUTION IS NECESSARY.
C
C     NOTE THAT THIS VERSION OF NUITSL REQUIRES THAT PW HAVE N**2 + 2*N
C     LOCATIONS SINCE 2*N LOCATIONS ARE USED BY THE IMSL LINEAR EQUATION
C     SOLVER.
C
C     NOTE THAT THE PARAMETERS EPS AND YMAX ARE USEFUL IF AN ITERATIVE
C     METHOD IS USED TO SOLVE THE SYSTEM OF EQUATIONS.
C
C     THE CALLING SEQUENCE FOR THIS SUBROUTINE IS
C
C     CALL NUITSL(PW,DY,F1,N,NY,EPS,YMAX,NEWPW,KRET)
```

```
C
C     WHERE THE PARAMETERS ARE DEFINED AS FOLLOWS.
C
C        PW       - THE J MATRIX CALCULATED IN SUBROUTINE JACMAT
C        DY       - THE RIGHT HAND SIDE OF THE LINEAR SYSTEM TO BE SOLVED
C        F1       - THE SOLUTION IS RETURNED IN THE ARRAY F1
C        N        - SAME AS IN LCASUB, TOTAL NUMBER OF VARIABLES
C        NY       - SAME AS IN LCASUB, NUMBER OF DIFFERENTIAL EQUATIONS
C                   AND NONLINEAR VARIABLES
C        EPS      - L2 ERROR CONSTANT USED IN LCASUB
C        YMAX     - MAXIMUM VALUES OF Y(I,I) SEEN UP TO THE CURRENT TIME
C        NEWPW    - INDICATES WHETHER A NEW J MATRIX HAS BEEN COMPUTED
C                      =1  INDICATES A NEW J MATRIX HAS BEEN COMPUTED
C                          SINCE THE LAST ENTRY TO NLITSL.  NEWPW
C                          SHOULD BE SET TO ZERO IF SOME PREPROCESSING
C                          SUCH AS LU DECOMPOSITION MUST BE DONE ON A
C                          NEW  J  MATRIX.
C                      =0  INDICATES THE J MATRIX IS THE SAME AS WHEN
C                          NLITSL WAS LAST ENTERED
C        KRET     - RETURN INDICATOR
C                      =0  NORMAL RETURN
C                      =1  ERROR RETURN.  SOLUTION OF EQUATIONS COULD
C                          NOT BE OBTAINED.
C
C     ------------------------------------------------------------------
      DIMENSION PW(1), DY(1), F1(1), YMAX(1)
      NL = N-NY
      IF (NEWPW.EQ.0) GO TO 100
      NEWPW = 0
      NN = N*N+1
      NNN = NN+N
      CALL LLOADF (PW,PW,N,N,0,D1,D2,PW(NN),PW(NNN),F1,IER)
      IF (IER.EQ.0) GO TO 100
      KRET = 1
      RETURN
  100 CALL LLELMF (PW,DY,PW(NN),N,N,F1)
      KRET = 0
      RETURN
      END
```


SAMPLE INPUT FILE FOR CASE 1
* (ZERO CELLPA LOCATION)
1
25
.1
20.0
0.0
5C.C
5C.0
14.7
1.4
.CC4
.005
1.C
.25
.34
.0
.9
7C.3
.231
.239
2.0
.01631
1050.0
Initial temperature of fibers (deg-F)
IELEM= 0, must input N.P. locations; 1, automatically divides domain into NNP-1 equilength elements.
NNP= number of nodal points.
T= time step of integration (sec.)
HMAX= maximum allowable time step (sec.)
TSTART= start time of problem, normally equal zero (sec.)
UINF1= exterior surface velocity (kt.)
TAMB= ambient temperature (deg F)
PAMB= ambient pressure (p.s.i.)
TORT= tortuosity
D1= filament diameter (inches)
SPACE1= ply thickness (inches)
HLENTH= reference length (equal to 1 ft.)
XLENT1= plate thickness (inches)
RGAS= gas constant for air (lbf*ft.per lbm*deg-R)
GCOND= bulk conductivity of graphite (btu per hr*ft*deg-F)
EMIS= fiber emissivity
ROG= bulk density of graphite (lbm per cu.ft.)
SPHTG= specific heat of graphite (btu per lbm*deg-F)
SPHTA= specific heat of air at constant pressure (btu per lbm*deg-F)
HSURFL= heat transfer coefficient at x=0 (btu per sq. ft*hr*deg-F)
CAMB1= ambient concentration of 02 (lbm per cu.ft.)

Initial temperature of air (deg-F)
Initial concentration of O2 (lbm per cu.ft.)

.004
.004

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